# wwPDB EM Map/Model Validation Report (i)

Jun 2, 2016 – 11:42 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 5IV5 |
| EMDB ID: | : | EMD-3374 |
| Title | : | Cryo-electron microscopy structure of the hexagonal pre-attachment T4 baseplate-tail tube complex |
| Authors | : | Taylor, N.M.I.; Guerrero-Ferreira, R.C.; Goldie, K.N.; Stahlberg, H.; Leiman, P.G. |
| Deposited on | : | 2016-03-19 |
| Resolution | : | 4.11 Å(reported) |
| Based on PDB ID | : | 4KU0, 1H6W, 1OCY, 1K28, 3H2T, 4HRZ, 1N7Z, 1S2E, 1EL6, 2FKK |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

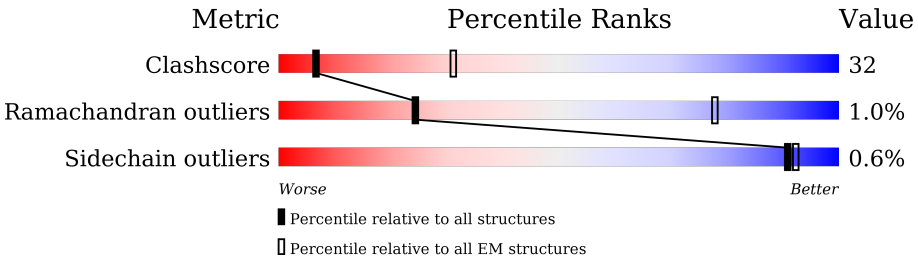
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20027674 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 660 | 46% 53% |
| 1 | B | 660 | 43% 53% |
| 1 | BH | 660 | 47% 52% |
| 1 | BI | 660 | 43% 54% |
| 1 | EA | 660 | 47% 53% |
| 1 | EB | 660 | 42% 54% |
| 1 | GD | 660 | 47% 52% |
| 1 | GE | 660 | 44% 53% |
| 1 | X | 660 | 47% 53% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | Y | 660 | 44% 53% |
| 1 | u | 660 | 99% |
| 1 | v | 660 | 96% |
| 2 | BJ | 1032 | 32% 60% |
| 2 | C | 1032 | 34% 59% |
| 2 | EC | 1032 | 32% 61% |
| 2 | GF | 1032 | 33% 60% |
| 2 | Z | 1032 | 35% 58% |
| 2 | w | 1032 | 92% 5% |
| 3 | CA | 334 | 50% 47% |
| 3 | CB | 334 | 55% 43% |
| 3 | D | 334 | 51% 47% |
| 3 | E | 334 | 56% 43% |
| 3 | ED | 334 | 49% 48% |
| 3 | EE | 334 | 55% 43% |
| 3 | GG | 334 | 50% 47% |
| 3 | GH | 334 | 56% 42% |
| 3 | a | 334 | 97% |
| 3 | b | 334 | 98% |
| 3 | x | 334 | 97% |
| 3 | y | 334 | 98% |
| 4 | AA | 288 | 59% 40% |
| 4 | AB | 288 | 61% 37% |
| 4 | CC | 288 | 58% 41% |
| 4 | CD | 288 | 56% 43% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | CE | 288 | 57% 42% |
| 4 | EF | 288 | 57% 42% |
| 4 | EG | 288 | 57% 42% |
| 4 | EH | 288 | 56% 43% |
| 4 | F | 288 | 59% 40% |
| 4 | G | 288 | 57% 42% |
| 4 | GI | 288 | 58% 41% |
| 4 | GJ | 288 | 57% 42% |
| 4 | H | 288 | 58% 41% |
| 4 | HA | 288 | 57% 42% |
| 4 | c | 288 | 99% |
| 4 | d | 288 | 99% |
| 4 | e | 288 | 99% |
| 4 | z | 288 | 99% |
| 5 | AC | 602 | 41% 55% |
| 5 | AD | 602 | 39% 57% |
| 5 | AE | 602 | 41% 55% |
| 5 | CF | 602 | 40% 57% |
| 5 | CG | 602 | 37% 59% |
| 5 | CH | 602 | 41% 55% |
| 5 | EI | 602 | 40% 56% |
| 5 | EJ | 602 | 38% 59% |
| 5 | FA | 602 | 40% 56% |
| 5 | HB | 602 | 40% 56% |
| 5 | HC | 602 | 38% 59% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | HD | 602 | 40% 56% |
| 5 | I | 602 | 40% 56% |
| 5 | J | 602 | 39% 57% |
| 5 | K | 602 | 41% 55% |
| 5 | f | 602 | 96% |
| 5 | g | 602 | 95% 5% |
| 5 | h | 602 | 95% 5% |
| 6 | AF | 219 | 51% 47% |
| 6 | AG | 219 | 57% 42% |
| 6 | AH | 219 | 56% 42% |
| 6 | CI | 219 | 52% 46% |
| 6 | CJ | 219 | 57% 42% |
| 6 | DA | 219 | 57% 42% |
| 6 | FB | 219 | 52% 46% |
| 6 | FC | 219 | 55% 43% |
| 6 | FD | 219 | 52% 47% |
| 6 | HE | 219 | 55% 43% |
| 6 | HF | 219 | 56% 42% |
| 6 | HG | 219 | 55% 44% |
| 6 | L | 219 | 53% 45% |
| 6 | M | 219 | 54% 44% |
| 6 | N | 219 | 52% 47% |
| 6 | i | 219 | 98% |
| 6 | j | 219 | 98% |
| 6 | k | 219 | 98% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 7 | AI | 527 | 41% 57% |
| 7 | AJ | 527 | 40% 59% |
| 7 | BA | 527 | 39% 59% |
| 7 | DB | 527 | 40% 58% |
| 7 | DC | 527 | 39% 59% |
| 7 | DD | 527 | 39% 59% |
| 7 | FE | 527 | 40% 59% |
| 7 | FF | 527 | 39% 61% |
| 7 | FG | 527 | 38% 60% |
| 7 | HH | 527 | 42% 57% |
| 7 | HI | 527 | 40% 59% |
| 7 | HJ | 527 | 39% 59% |
| 7 | O | 527 | 40% 58% |
| 7 | P | 527 | 39% 60% |
| 7 | Q | 527 | 39% 59% |
| 7 | l | 527 | 98% |
| 7 | m | 527 | 98% |
| 7 | n | 527 | 98% |
| 8 | BB | 163 | 47% 53% |
| 8 | BC | 163 | 47% 53% |
| 8 | DE | 163 | 46% 53% |
| 8 | DF | 163 | 44% 56% |
| 8 | FH | 163 | 45% 54% |
| 8 | FI | 163 | 44% 55% |
| 8 | IA | 163 | 45% 54% |

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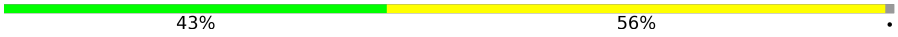
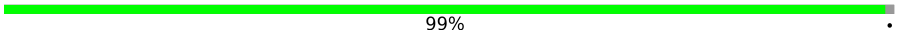
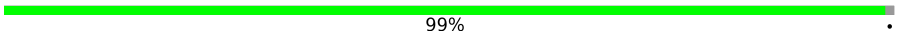
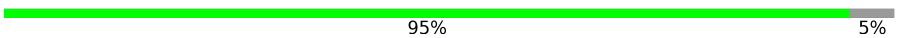
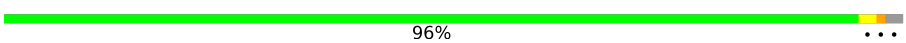
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | IB | 163 |   |
| 8 | R | 163 | |
| 8 | S | 163 | |
| 8 | o | 163 |   |
| 8 | p | 163 |   |
| 9 | BD | 132 | |
| 9 | DG | 132 | |
| 9 | FJ | 132 | |
| 9 | IC | 132 | |
| 9 | T | 132 | |
| 9 | q | 132 |   |
| 10 | BE | 364 | |
| 10 | DH | 364 | |
| 10 | GA | 364 | |
| 10 | ID | 364 | |
| 10 | U | 364 | |
| 10 | r | 364 | |
| 11 | BF | 196 | |
| 11 | DI | 196 | |
| 11 | GB | 196 | |
| 11 | IE | 196 | |
| 11 | V | 196 | |
| 11 | s | 196 |   |
| 12 | BG | 320 | |
| 12 | DJ | 320 | |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 12 | GC | 320 | 24% 35% 40% |
| 12 | IF | 320 | 24% 36% 40% |
| 12 | W | 320 | 27% 33% 40% |
| 12 | t | 320 | 58% 40% |
| 13 | YA | 575 | 49% 41% 6% |
| 13 | YB | 575 | 49% 41% 6% |
| 13 | YC | 575 | 48% 42% 6% |
| 14 | YD | 391 | 40% 47% 6% 7% |
| 14 | YE | 391 | 38% 48% 6% 7% |
| 14 | YF | 391 | 38% 48% 6% 7% |
| 15 | ZA | 97 | 76% 22% |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 549576 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Baseplate wedge protein gp6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | B | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |
| 1 | X | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | Y | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |
| 1 | u | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | v | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |
| 1 | BH | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | BI | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |
| 1 | EA | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | EB | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |
| 1 | GD | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5235 | 3308 | 867 | 1050 | 10 | | |
| 1 | GE | 648 | Total | C | N | O | S | 0 | 0 |
| | | | 5157 | 3259 | 854 | 1034 | 10 | | |

- Molecule 2 is a protein called Baseplate wedge protein gp7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |
| 2 | Z | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |
| 2 | w | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | BJ | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |
| 2 | EC | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |
| 2 | GF | 1004 | Total | C | N | O | S | 0 | 0 |
| | | | 8199 | 5247 | 1347 | 1578 | 27 | | |

- Molecule 3 is a protein called Baseplate wedge protein gp8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | E | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |
| 3 | a | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | b | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |
| 3 | x | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | y | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |
| 3 | CA | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | CB | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |
| 3 | ED | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | EE | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |
| 3 | GG | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2631 | 1677 | 430 | 507 | 17 | | |
| 3 | GH | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2658 | 1692 | 434 | 515 | 17 | | |

- Molecule 4 is a protein called Baseplate wedge protein gp9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | F | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | G | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | H | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | c | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | d | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | e | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | z | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | AA | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | AB | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | CC | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | CD | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | CE | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | EF | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | EG | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | EH | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | GI | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | GJ | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |
| 4 | HA | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1354 | 366 | 446 | 9 | | |

- Molecule 5 is a protein called Baseplate wedge protein gp10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | I | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | J | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | K | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | f | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | g | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | h | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | AC | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | AD | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | AE | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | CF | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | CG | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | CH | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | EI | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | EJ | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | FA | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | HB | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | HC | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |
| 5 | HD | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4675 | 2933 | 779 | 953 | 10 | | |

- Molecule 6 is a protein called Baseplate wedge protein gp11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | L | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | M | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | N | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | i | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | j | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | k | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | AF | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | AG | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | AH | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | CI | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | CJ | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | DA | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | FB | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | FC | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | FD | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | HE | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | HF | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |
| 6 | HG | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1056 | 273 | 334 | 2 | | |

- Molecule 7 is a protein called Short tail fiber protein gp12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | O | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | P | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | Q | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | l | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | m | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | n | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | AI | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | AJ | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | BA | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | DB | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | DC | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | DD | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | FE | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | FF | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | FG | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | HH | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | HI | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |
| 7 | HJ | 526 | Total | C | N | O | S | 0 | 0 |
| | | | 3945 | 2429 | 702 | 803 | 11 | | |

- Molecule 8 is a protein called Tail tube protein gp19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | R | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | S | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | o | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | p | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | BB | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | BC | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | DE | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | DF | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | FH | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | FI | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | IA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 8 | IB | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |

- Molecule 9 is a protein called Baseplate wedge protein gp25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | T | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |
| 9 | q | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |
| 9 | BD | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |
| 9 | DG | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |
| 9 | FJ | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |
| 9 | IC | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 636 | 169 | 202 | 4 | | |

- Molecule 10 is a protein called Baseplate tail-tube protein gp48.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | U | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |
| 10 | r | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |
| 10 | BE | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |
| 10 | DH | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |
| 10 | GA | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | ID | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1317 | 846 | 219 | 247 | 5 | | |

- Molecule 11 is a protein called Baseplate wedge protein gp53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | V | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |
| 11 | s | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |
| 11 | BF | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |
| 11 | DI | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |
| 11 | GB | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |
| 11 | IE | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1035 | 259 | 299 | 6 | | |

- Molecule 12 is a protein called Baseplate tail-tube protein gp54.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | W | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |
| 12 | t | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |
| 12 | BG | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |
| 12 | DJ | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |
| 12 | GC | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |
| 12 | IF | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1524 | 955 | 257 | 301 | 11 | | |

- Molecule 13 is a protein called Peptidoglycan hydrolase gp5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | YA | 554 | Total | C | N | O | S | 554 | 0 |
| | | | 25692 | 15942 | 4536 | 5088 | 126 | | |
| 13 | YB | 554 | Total | C | N | O | S | 554 | 0 |
| | | | 25692 | 15942 | 4536 | 5088 | 126 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | YC | 554 | Total<br>25692 | C<br>15942 | N<br>4536 | O<br>5088 | S<br>126 | 554 | 0 |

- Molecule 14 is a protein called Baseplate hub protein gp27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | YD | 364 | Total<br>17472 | C<br>11148 | N<br>2868 | O<br>3354 | S<br>102 | 364 | 0 |
| 14 | YE | 364 | Total<br>17472 | C<br>11148 | N<br>2868 | O<br>3354 | S<br>102 | 364 | 0 |
| 14 | YF | 364 | Total<br>17472 | C<br>11148 | N<br>2868 | O<br>3354 | S<br>102 | 364 | 0 |

- Molecule 15 is a protein called Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | ZA | 96 | Total<br>4254 | C<br>2682 | N<br>720 | O<br>834 | S<br>18 | 96 | 0 |

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 16 | AI | 1 | Total<br>1 | Zn<br>1 | 0 |
| 16 | FE | 1 | Total<br>1 | Zn<br>1 | 0 |
| 16 | O | 1 | Total<br>1 | Zn<br>1 | 0 |
| 16 | l | 1 | Total<br>1 | Zn<br>1 | 0 |
| 16 | HH | 1 | Total<br>1 | Zn<br>1 | 0 |
| 16 | DB | 1 | Total<br>1 | Zn<br>1 | 0 |

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

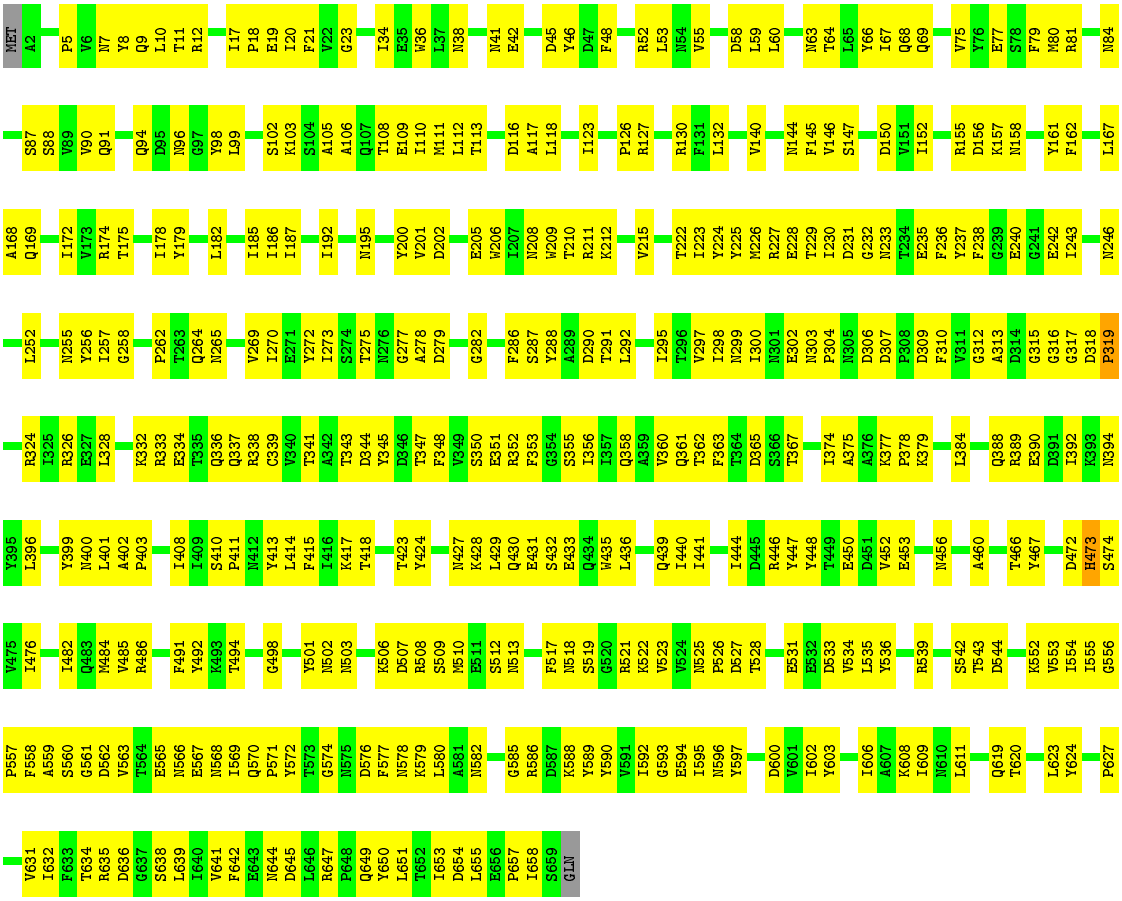
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 17 | ZA | 1 | Total<br>6 | Fe<br>6 | 1 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

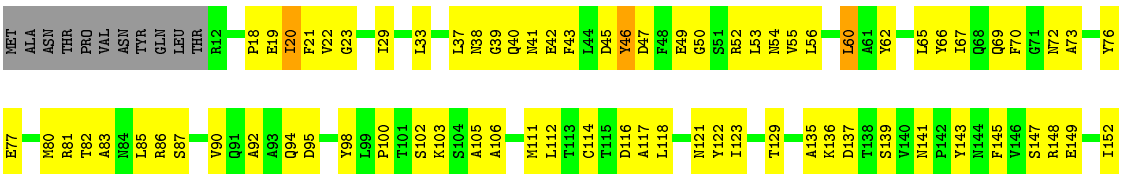
- Molecule 1: Baseplate wedge protein gp6

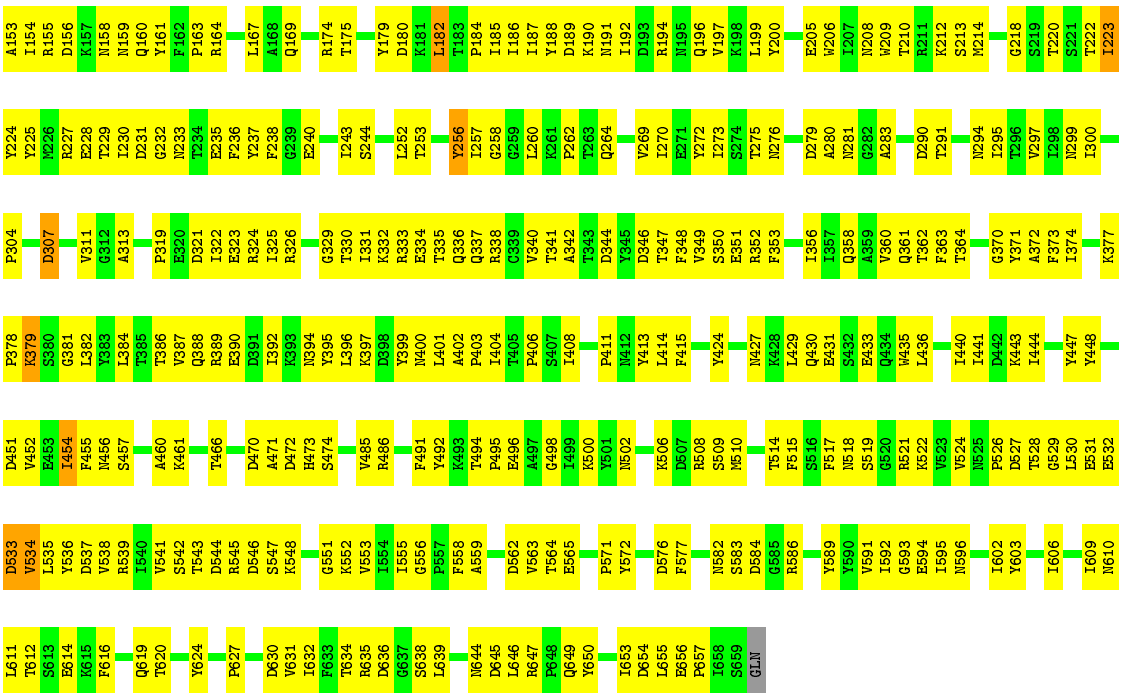
Chain A:




- Molecule 1: Baseplate wedge protein gp6

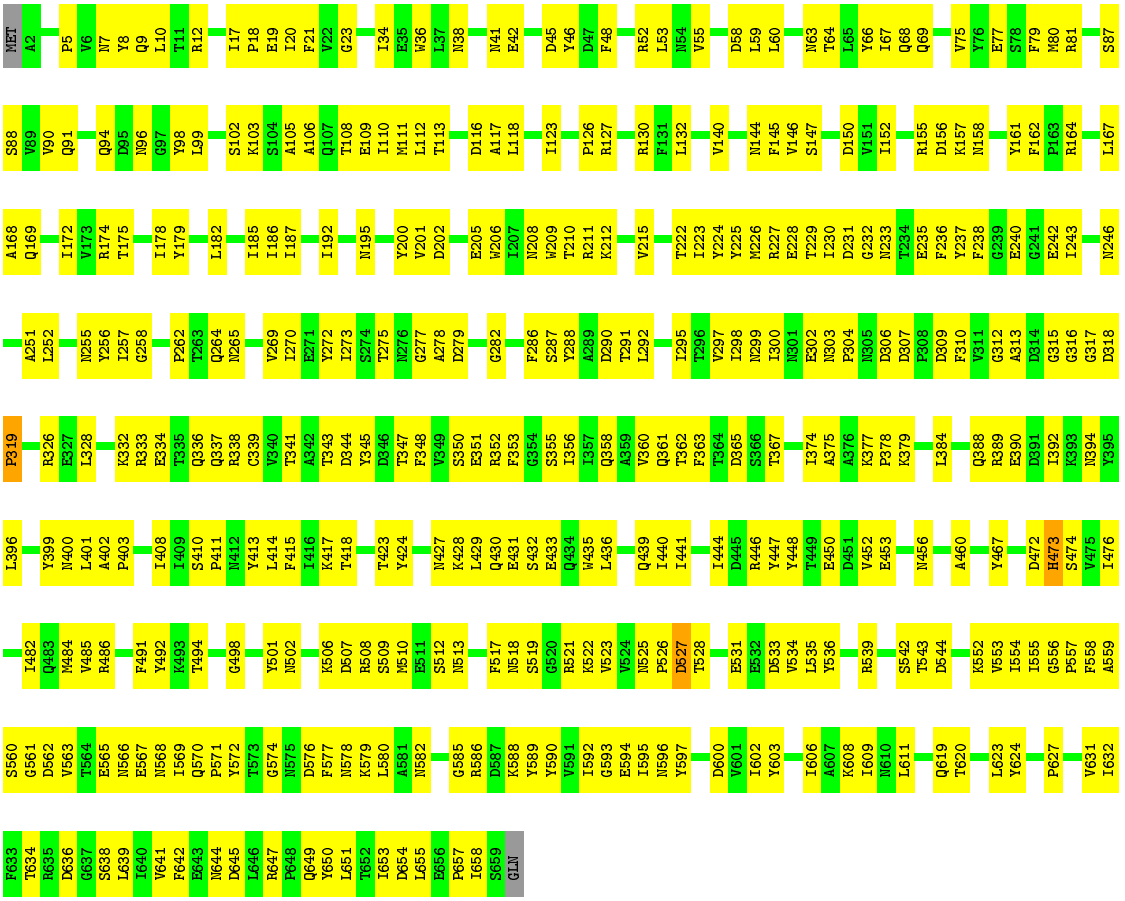
Chain B:





• Molecule 1: Baseplate wedge protein gp6

Chain X:



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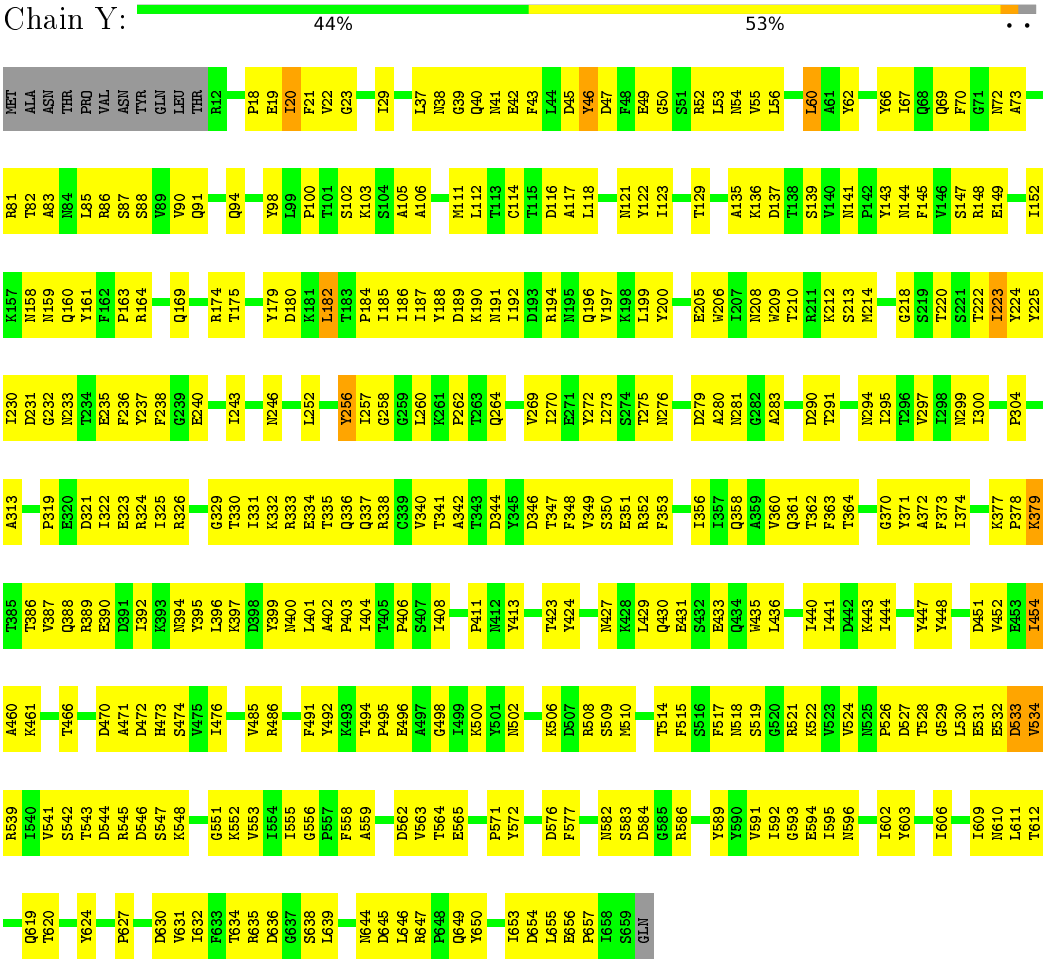
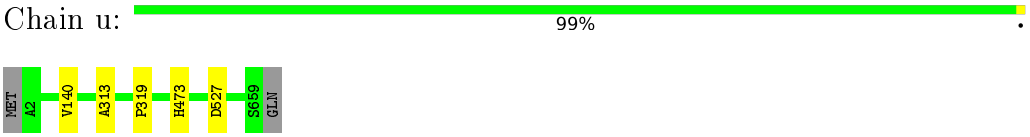
• Molecule 1: Baseplate wedge protein gp6

Chain Y:



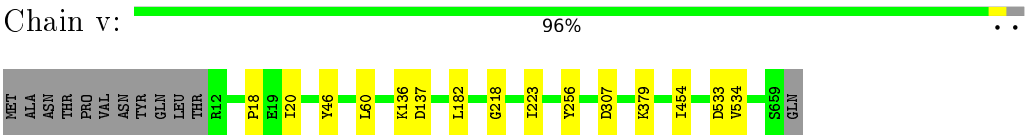

• Molecule 1: Baseplate wedge protein gp6

Chain u:



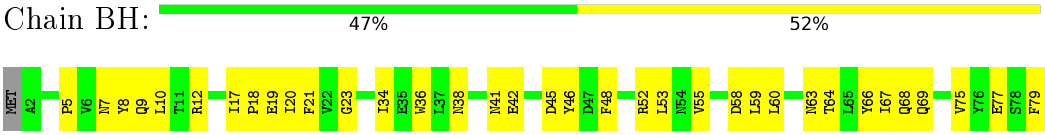

• Molecule 1: Baseplate wedge protein gp6

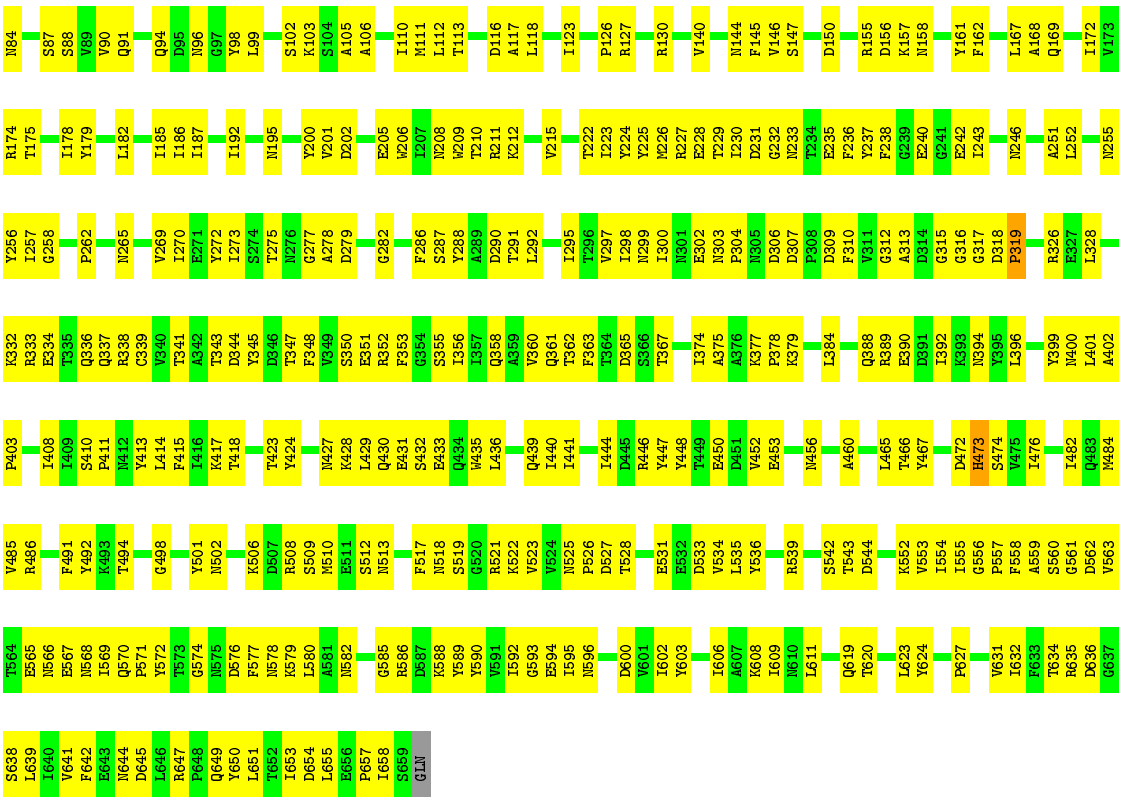
Chain v:




• Molecule 1: Baseplate wedge protein gp6

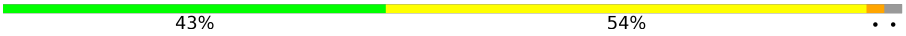
Chain BH:

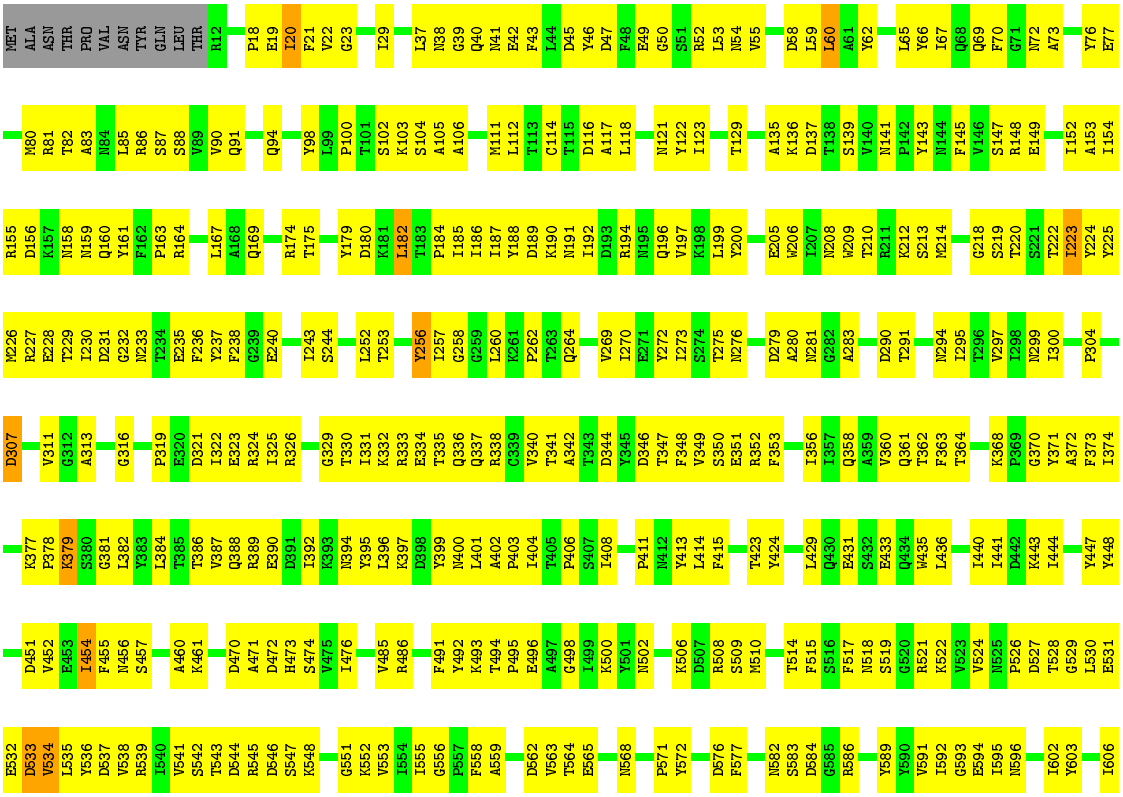




• Molecule 1: Baseplate wedge protein gp6

Chain BI:



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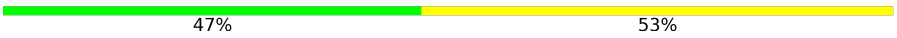
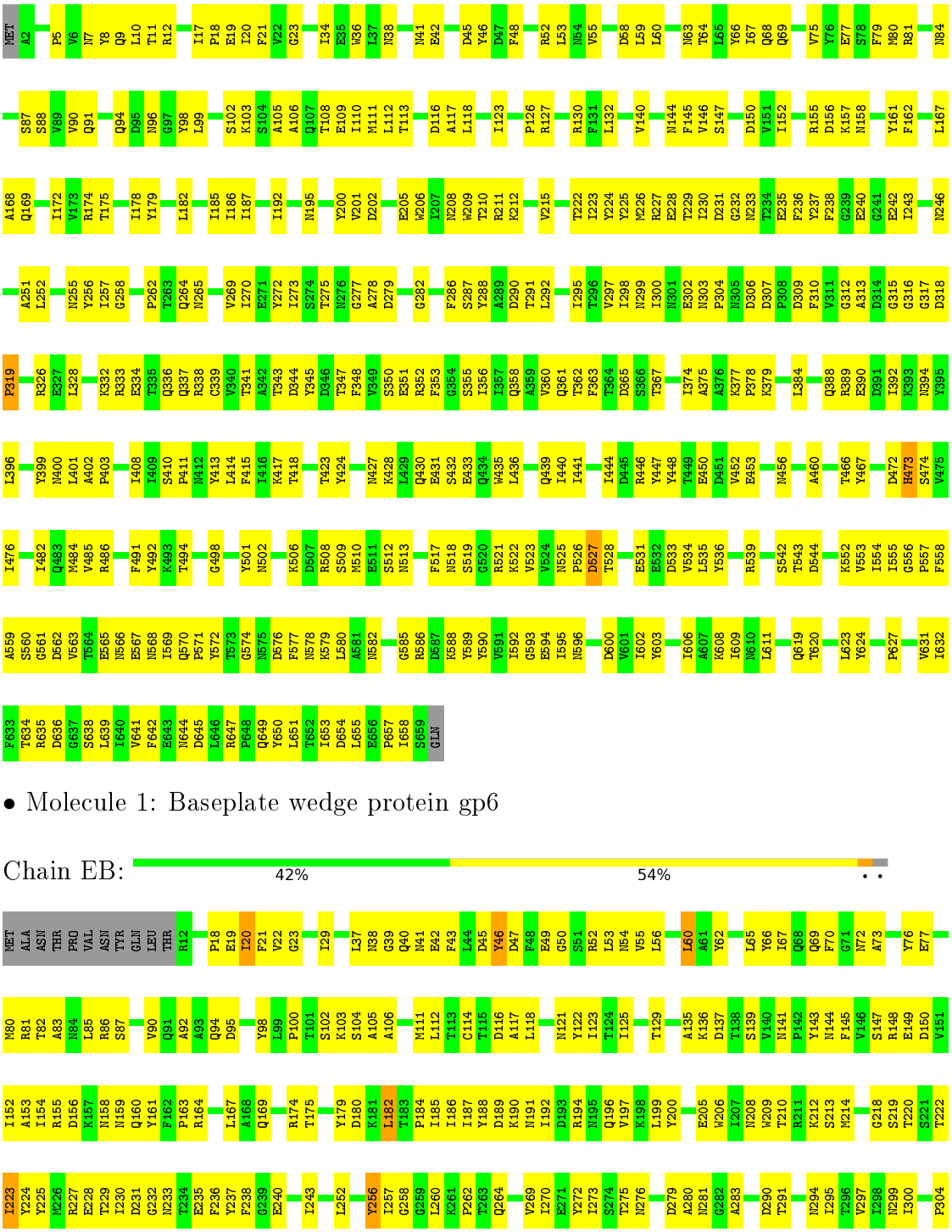
• Molecule 1: Baseplate wedge protein gp6

Chain EA:



• Molecule 1: Baseplate wedge protein gp6

Chain EB:



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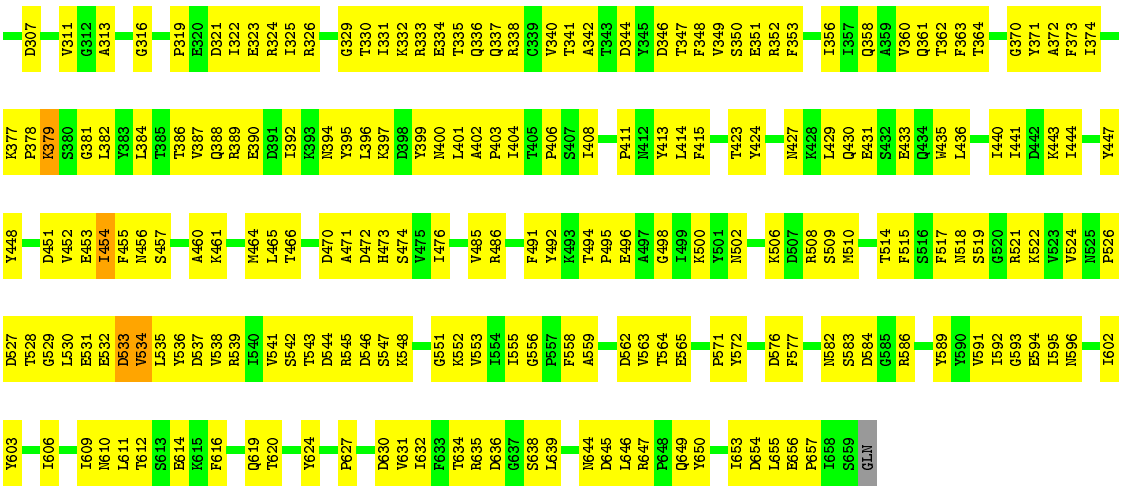
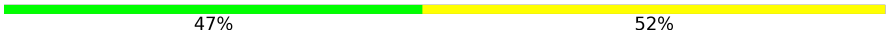
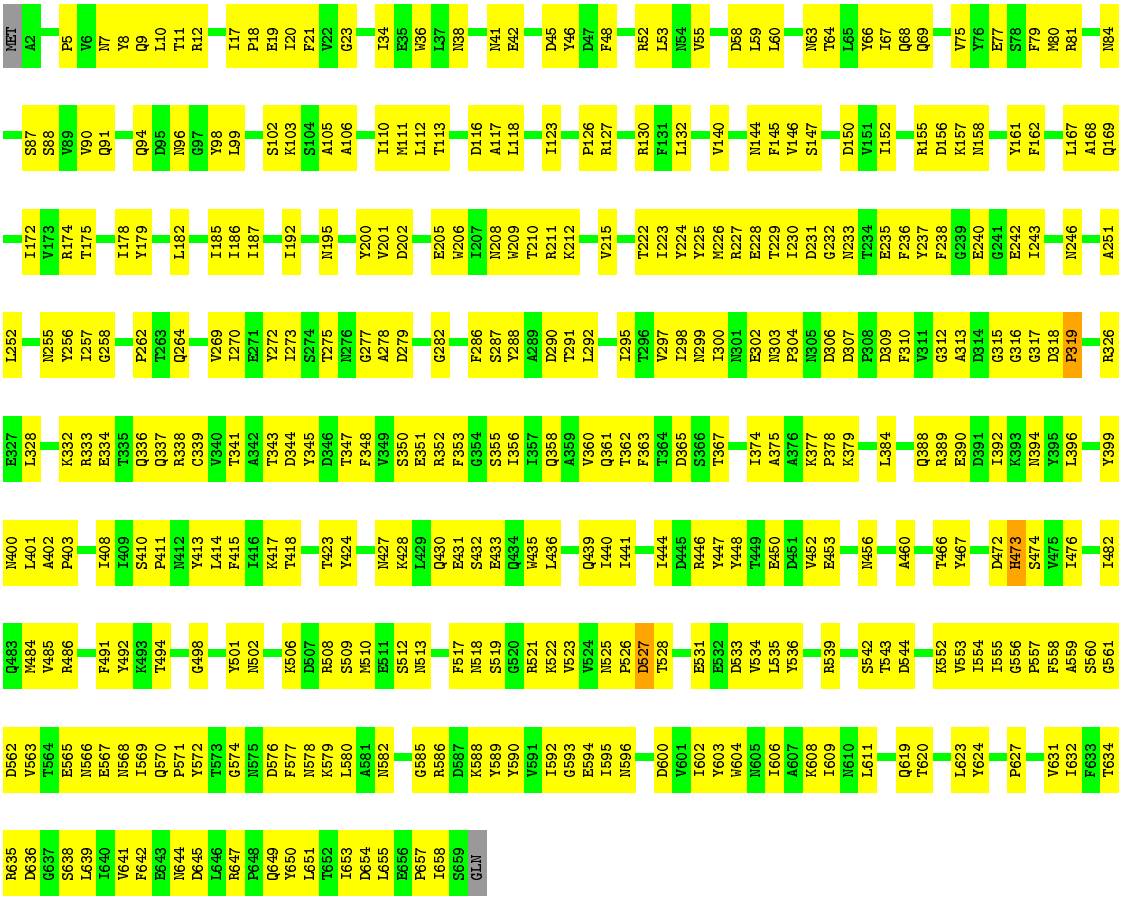


• Molecule 1: Baseplate wedge protein gp6

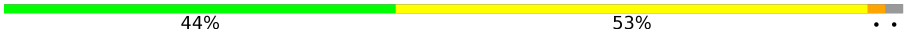
Chain GD:

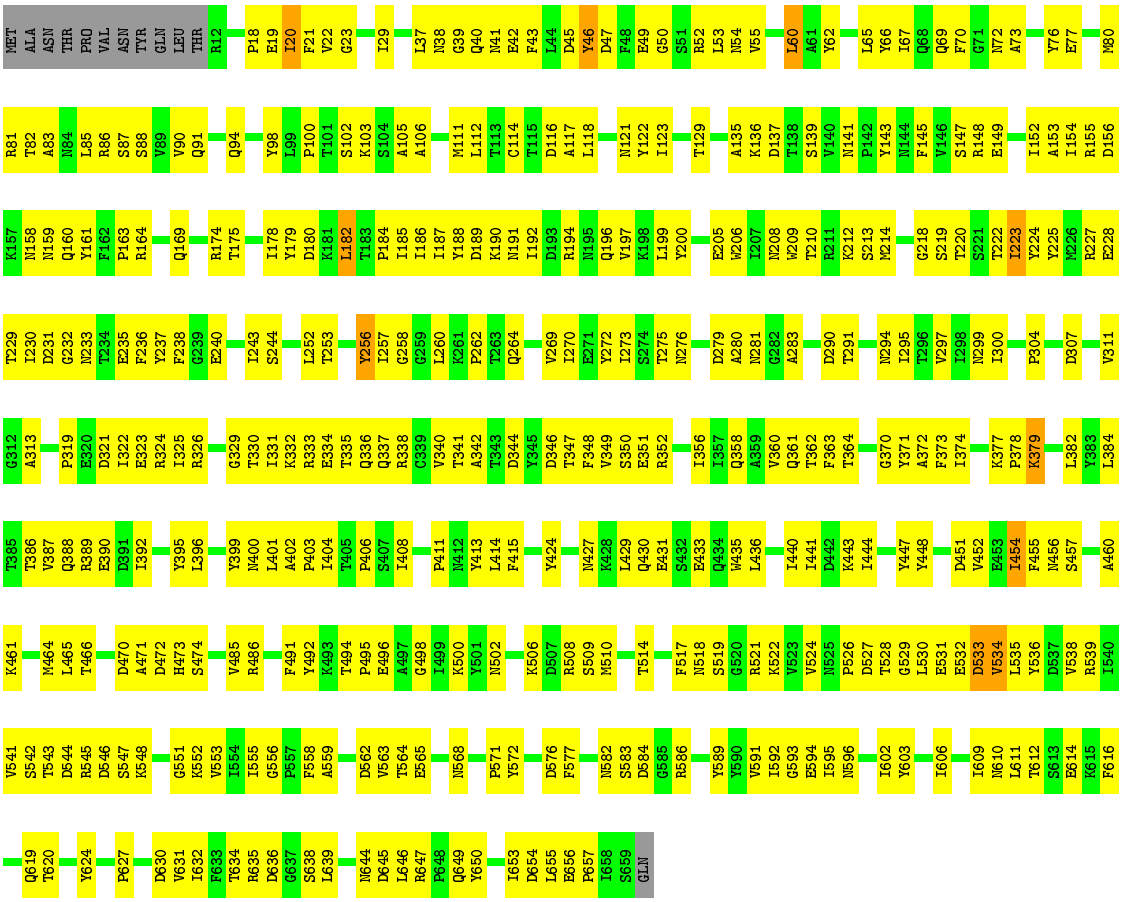


• Molecule 1: Baseplate wedge protein gp6

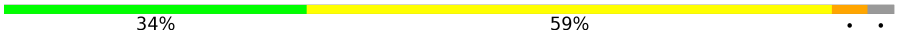
Chain GE:

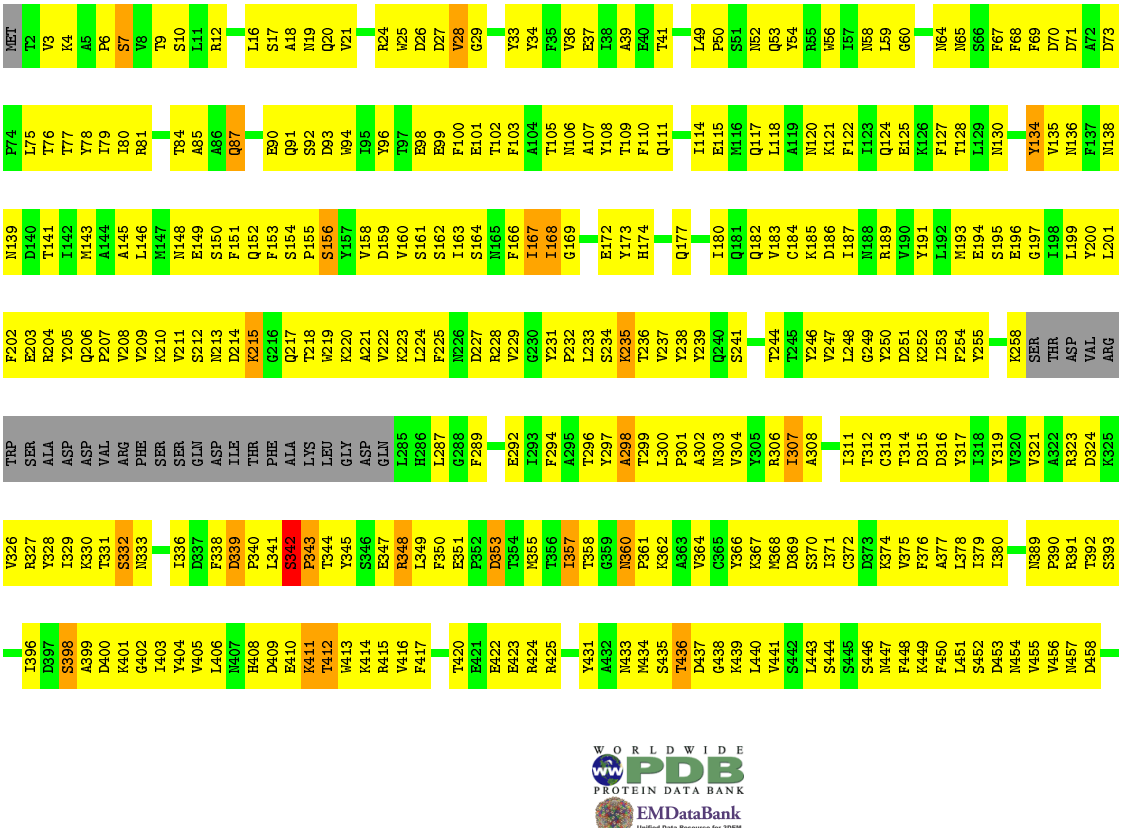




• Molecule 2: Baseplate wedge protein gp7

Chain C:



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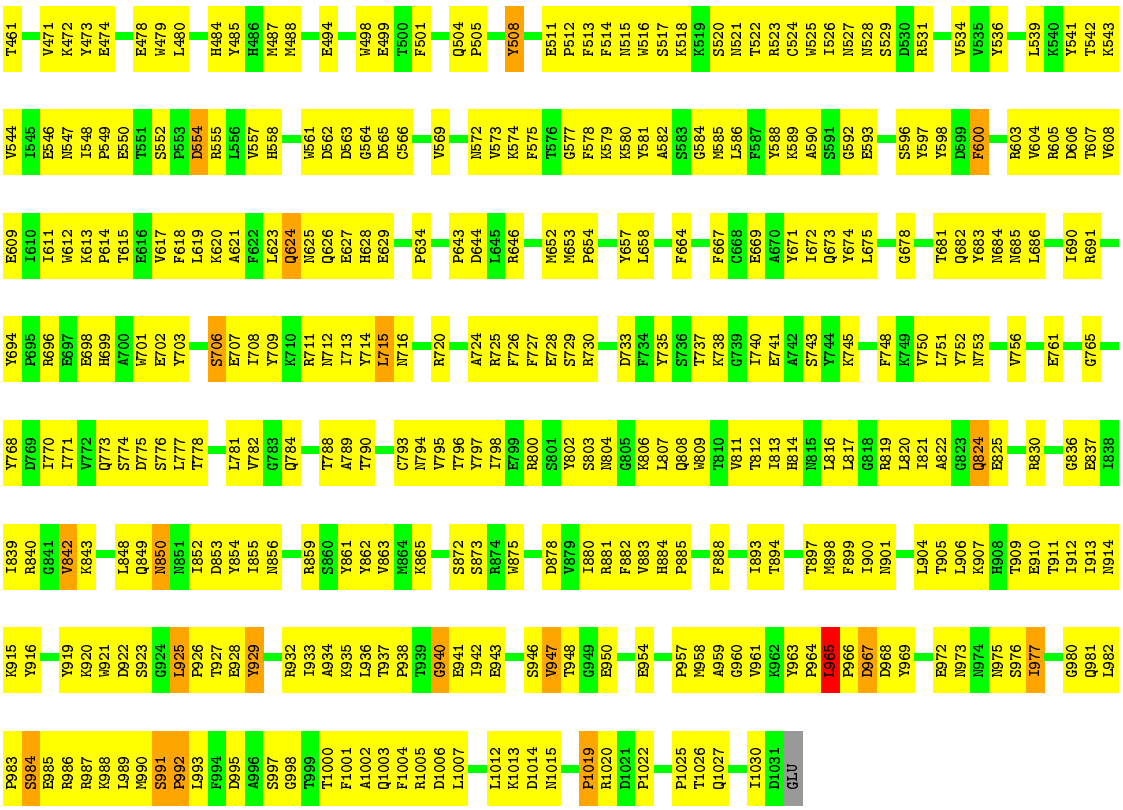
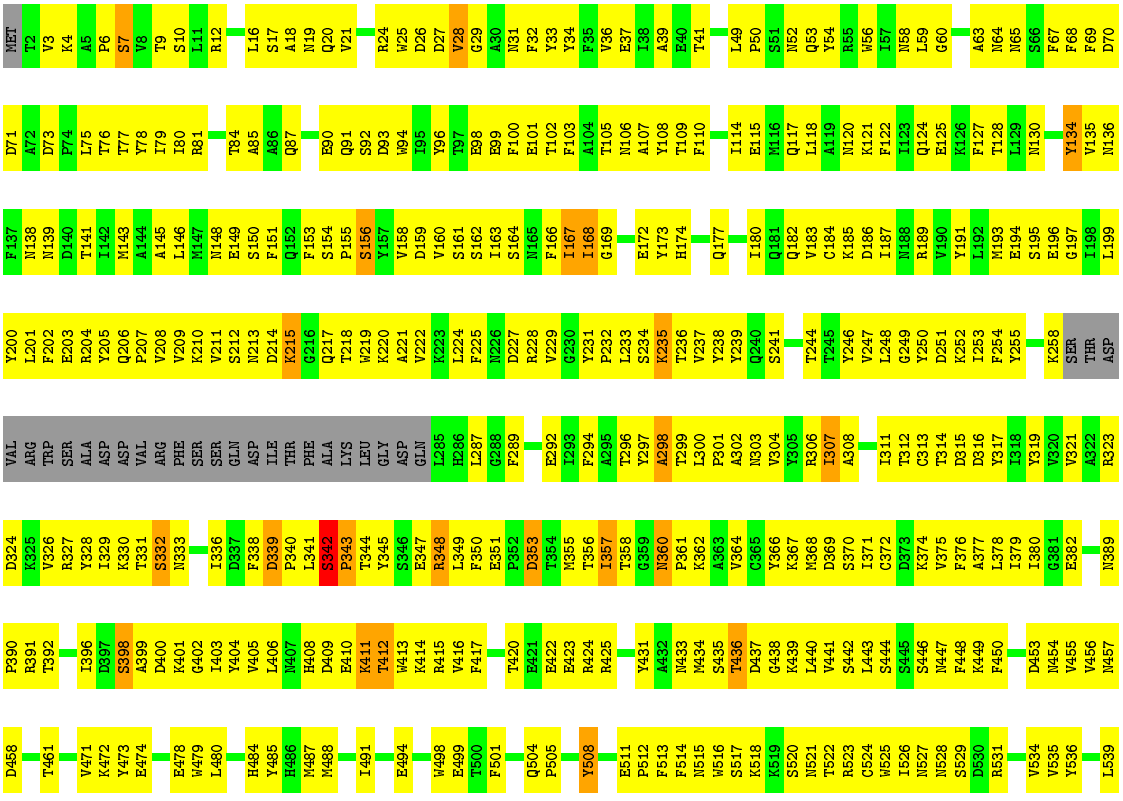


• Molecule 2: Baseplate wedge protein gp7

Chain Z:



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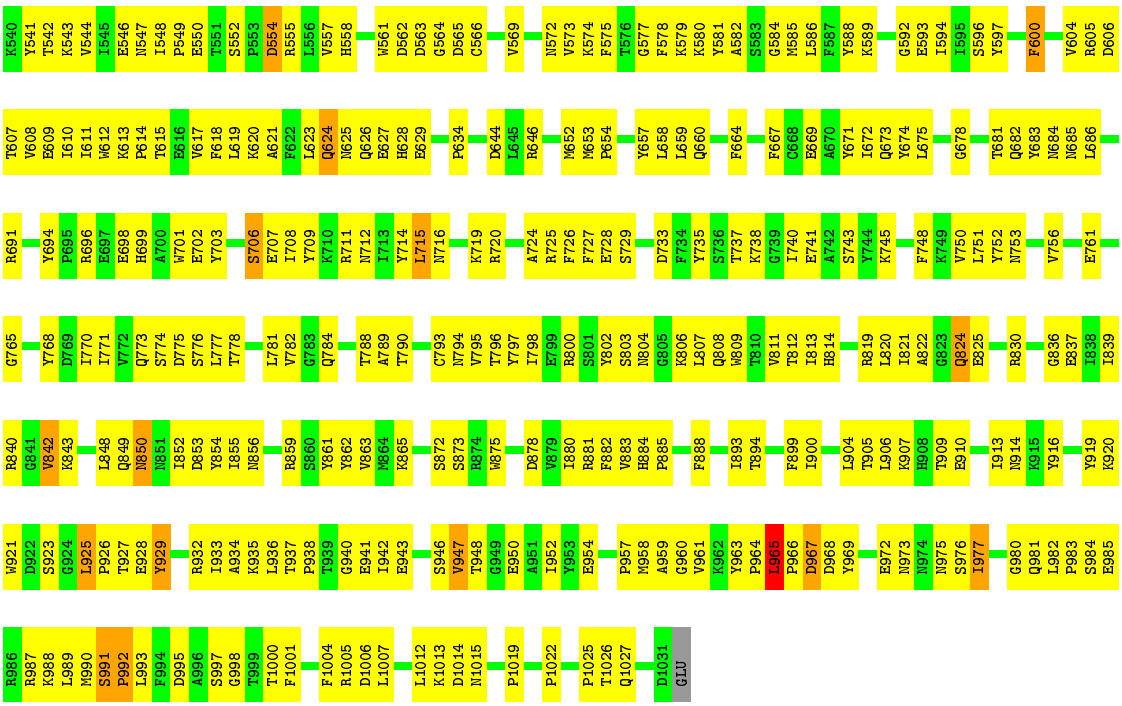
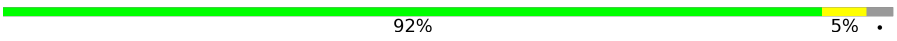
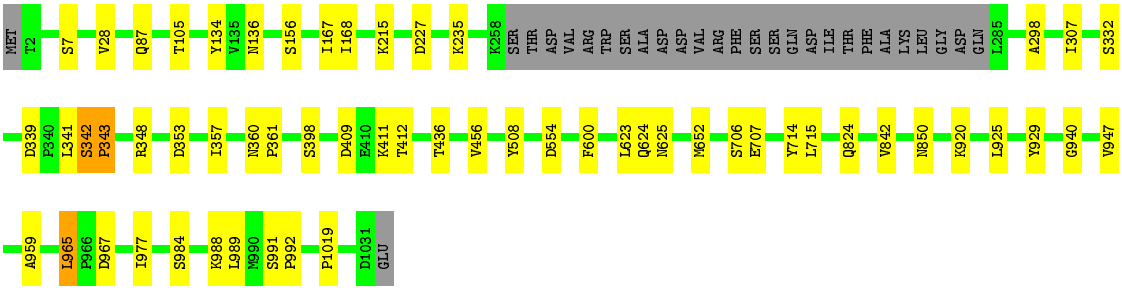


• Molecule 2: Baseplate wedge protein gp7

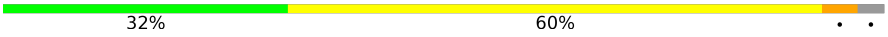
Chain w:

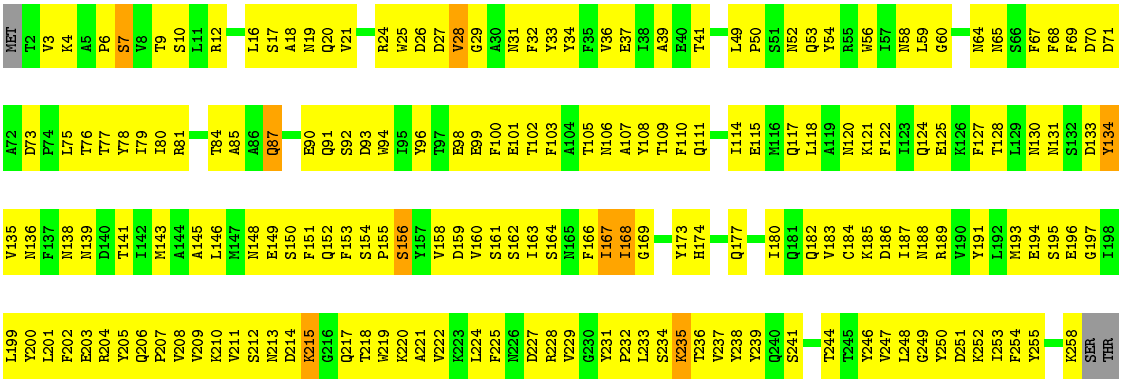


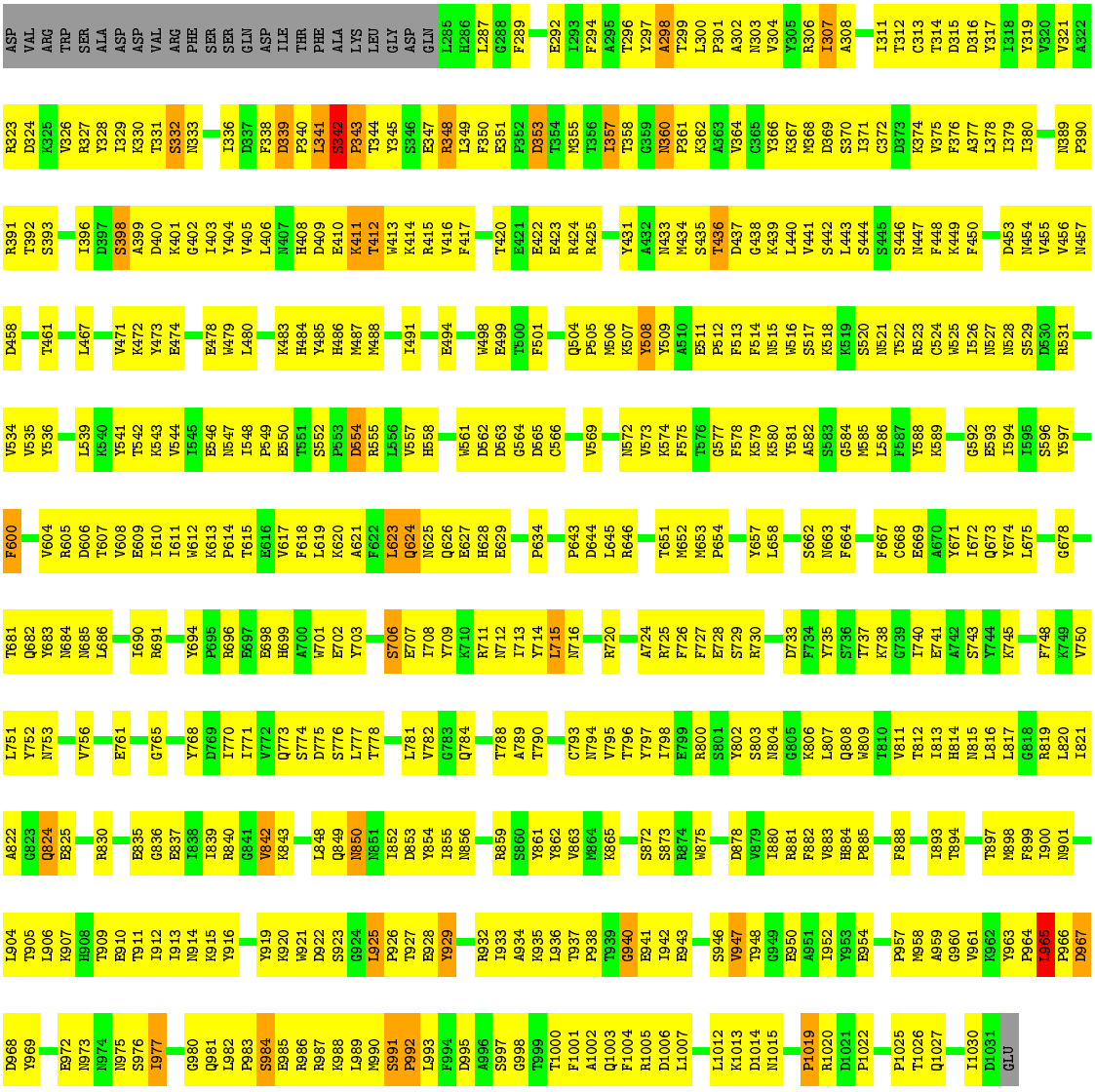



• Molecule 2: Baseplate wedge protein gp7

Chain BJ:

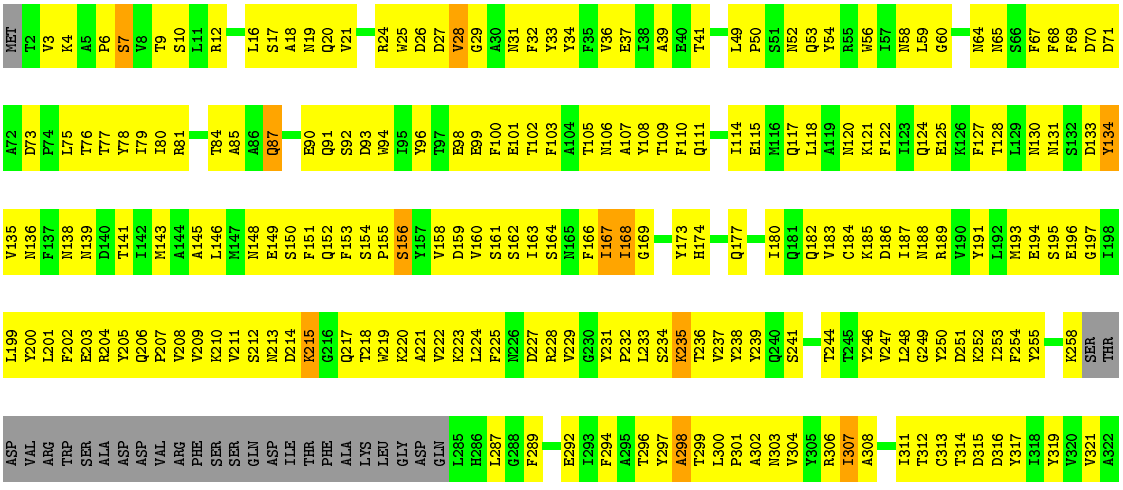


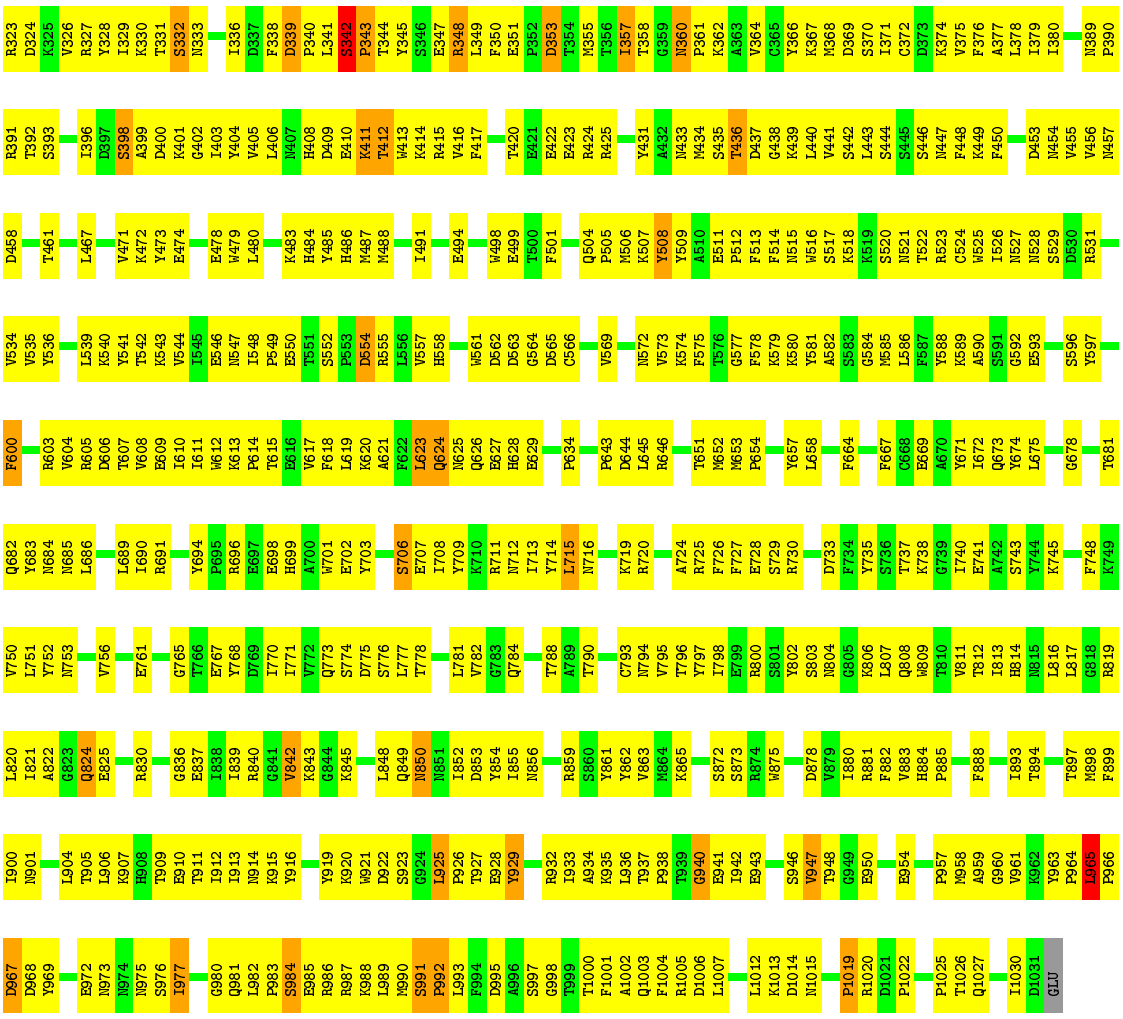


• Molecule 2: Baseplate wedge protein gp7

Chain EC:

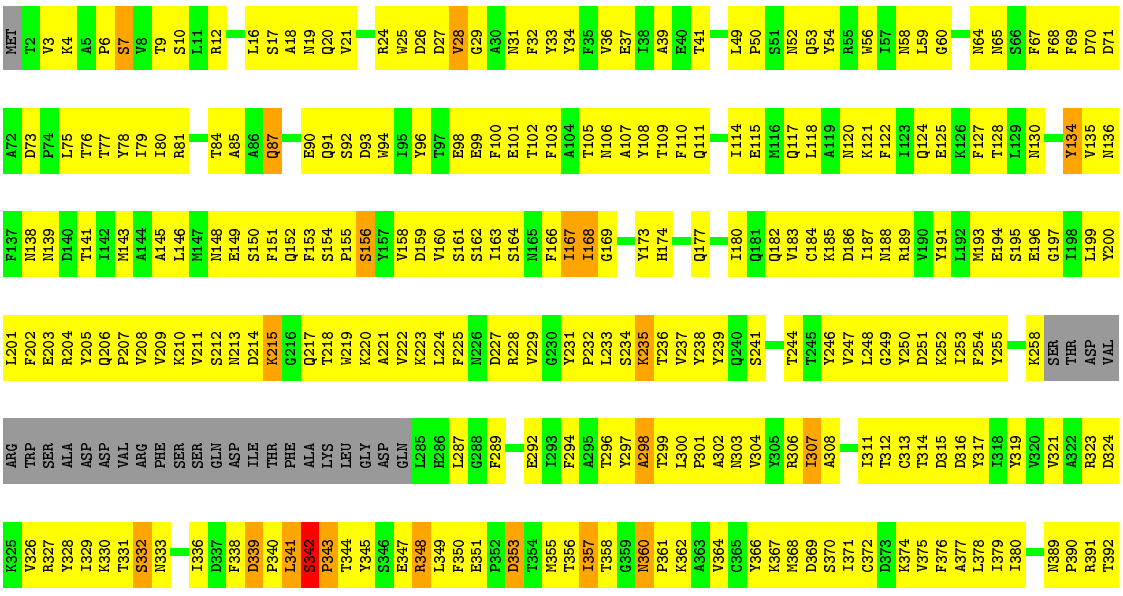


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



• Molecule 2: Baseplate wedge protein gp7

Chain GF:



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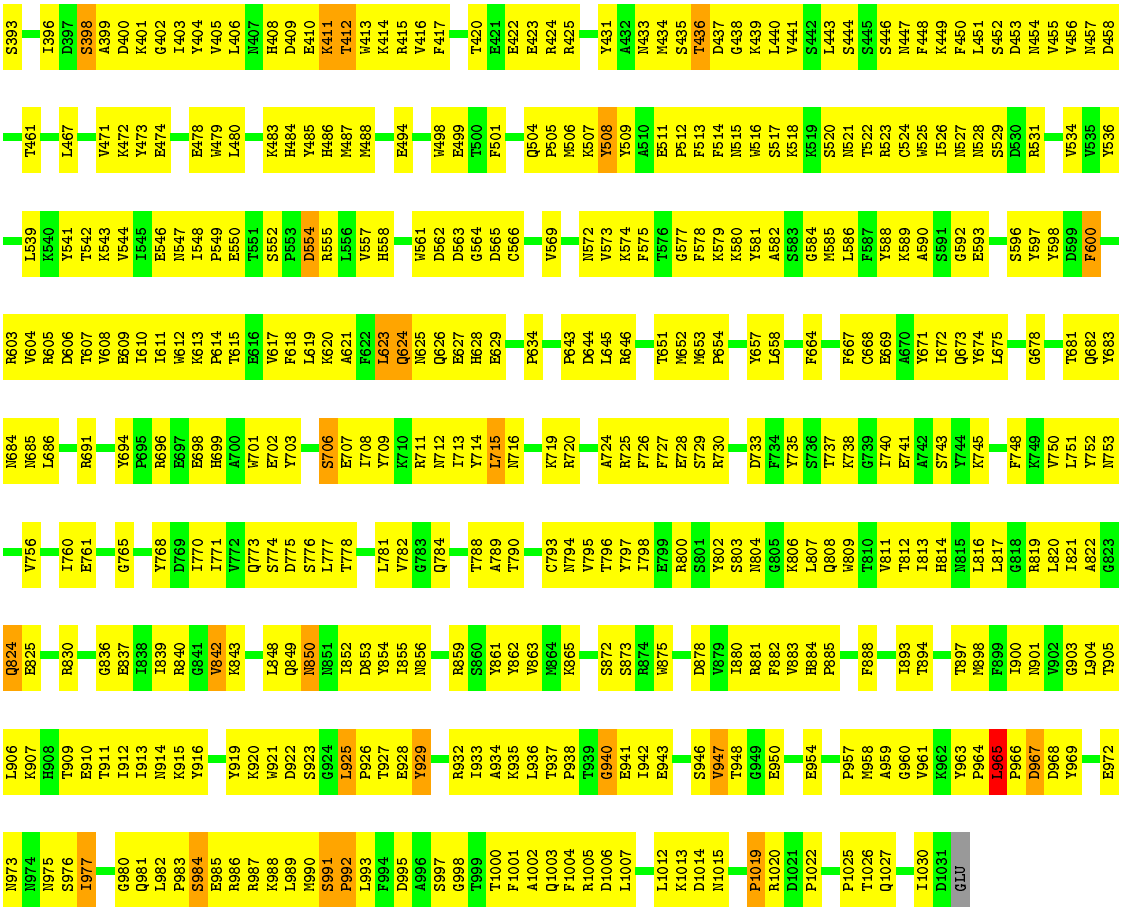
EMDataBank Unified Data Resource for 3DEM



• Molecule 3: Baseplate wedge protein gp8

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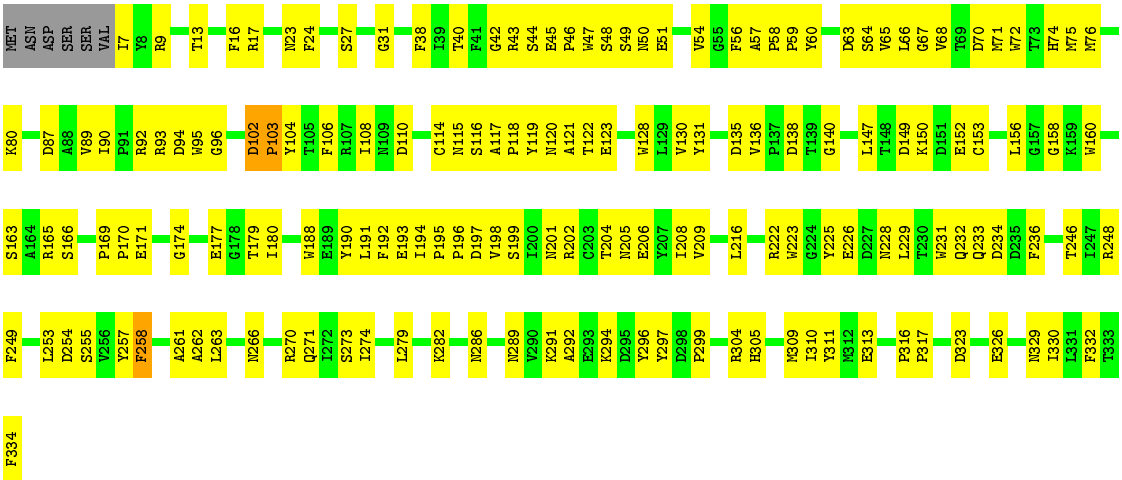
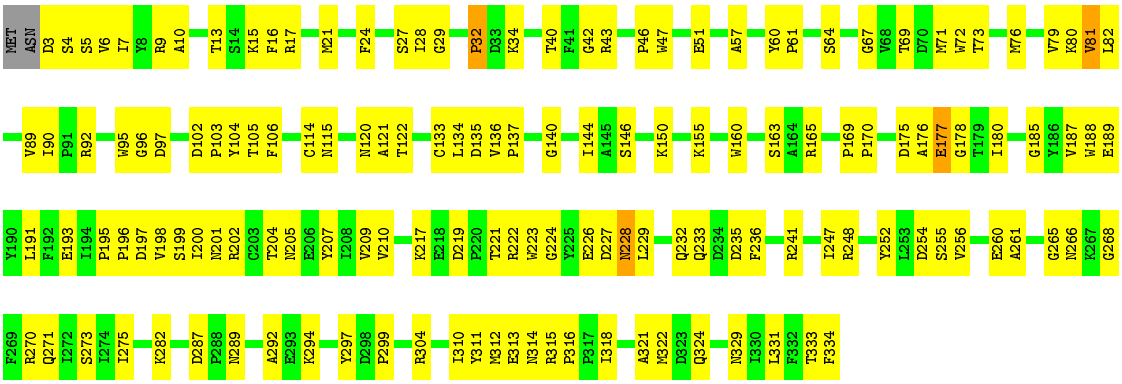


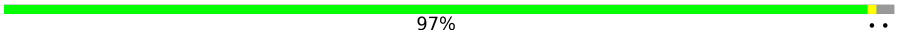
• Molecule 3: Baseplate wedge protein gp8

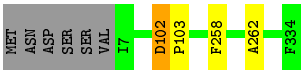
Chain E:




• Molecule 3: Baseplate wedge protein gp8

Chain a:




• Molecule 3: Baseplate wedge protein gp8

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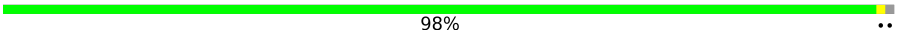
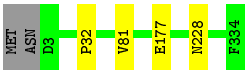
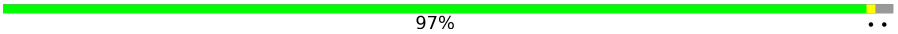
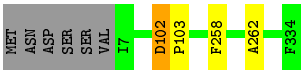



• Molecule 3: Baseplate wedge protein gp8

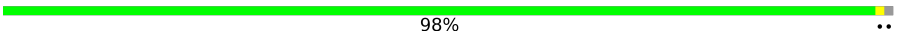
Chain x:

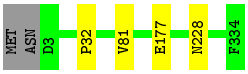



• Molecule 3: Baseplate wedge protein gp8

Chain y:




• Molecule 3: Baseplate wedge protein gp8

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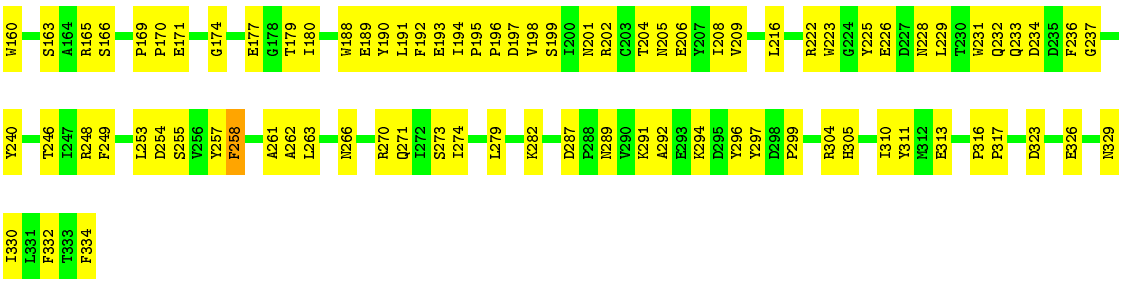


• Molecule 3: Baseplate wedge protein gp8

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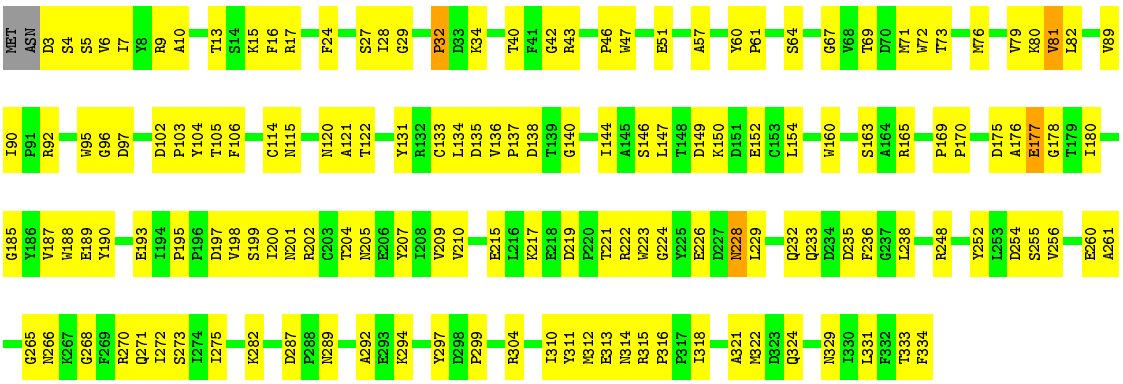


• Molecule 3: Baseplate wedge protein gp8

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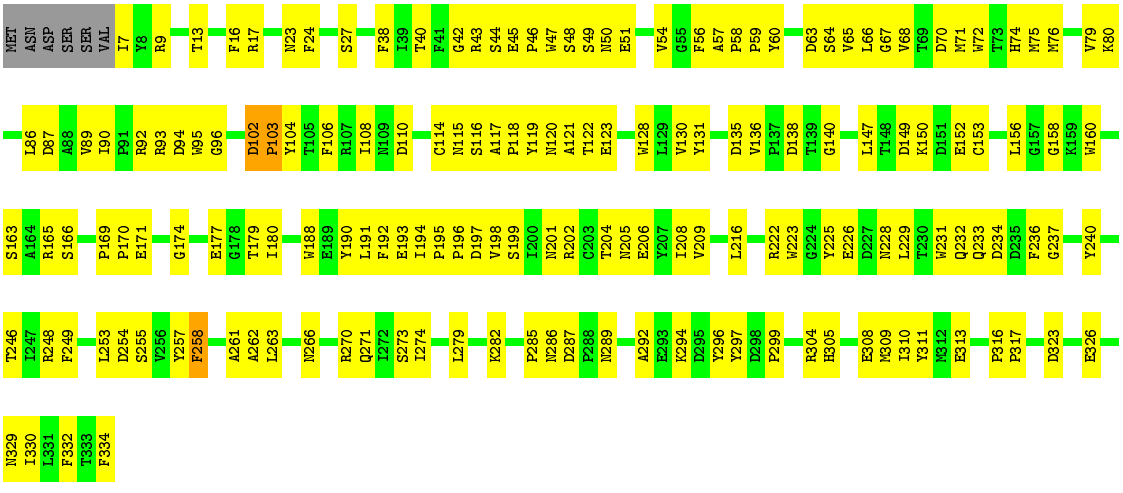


• Molecule 3: Baseplate wedge protein gp8

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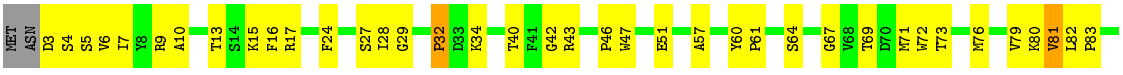

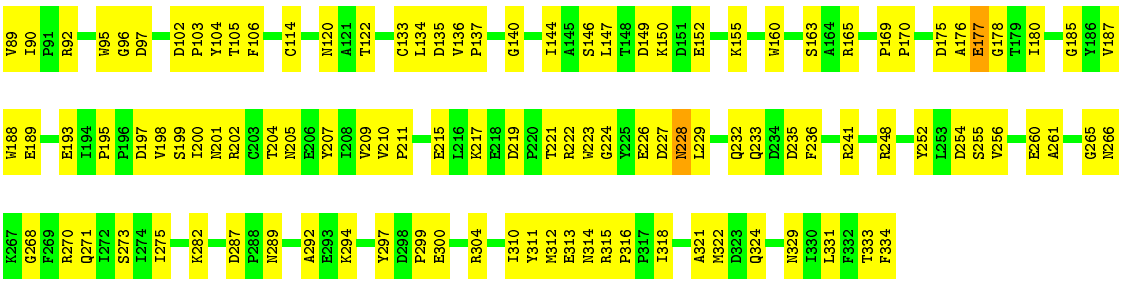

• Molecule 3: Baseplate wedge protein gp8

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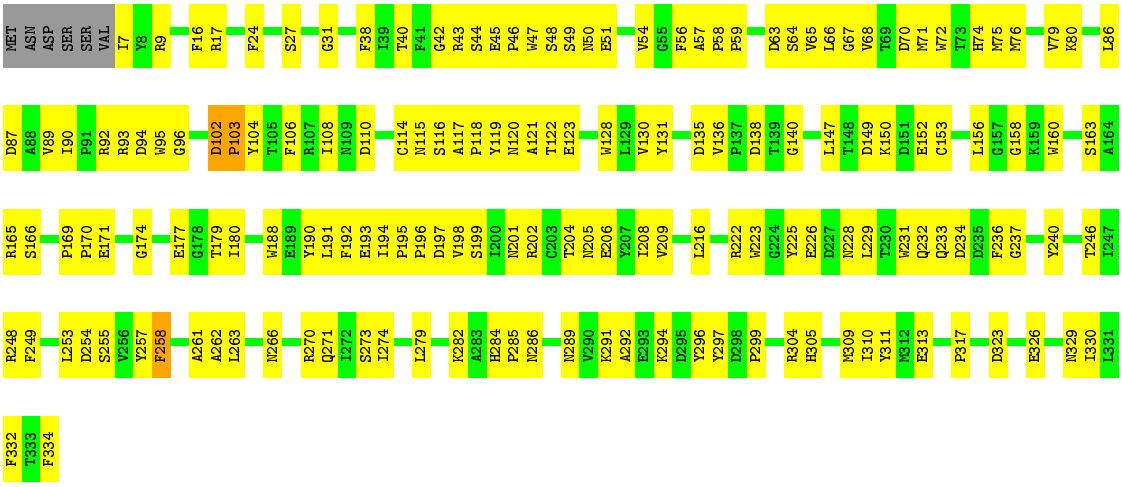
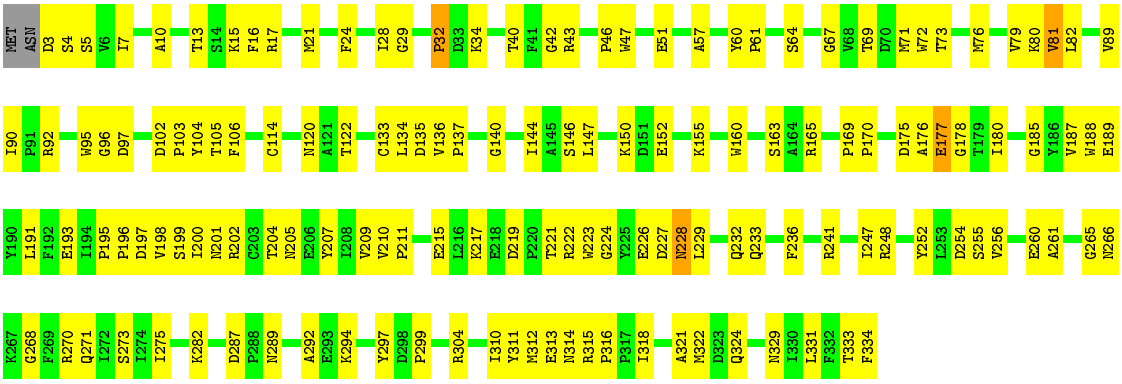


• Molecule 3: Baseplate wedge protein gp8

Chain GH:



• Molecule 4: Baseplate wedge protein gp9

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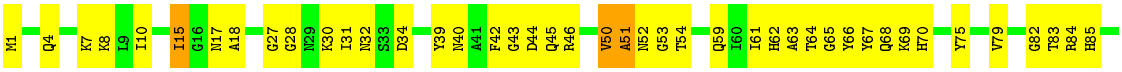

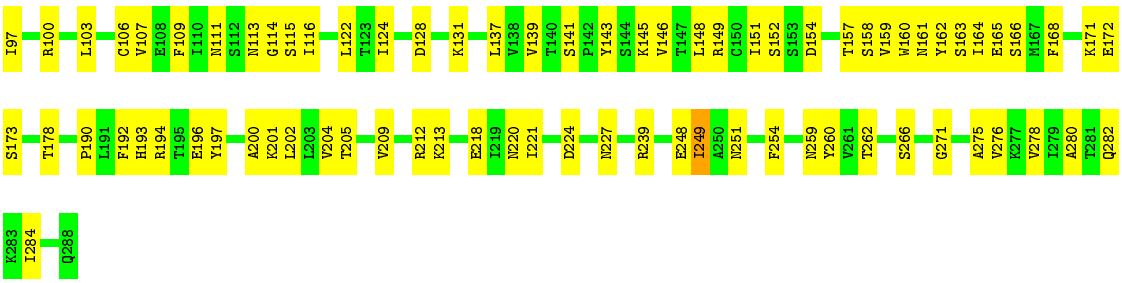


• Molecule 4: Baseplate wedge protein gp9

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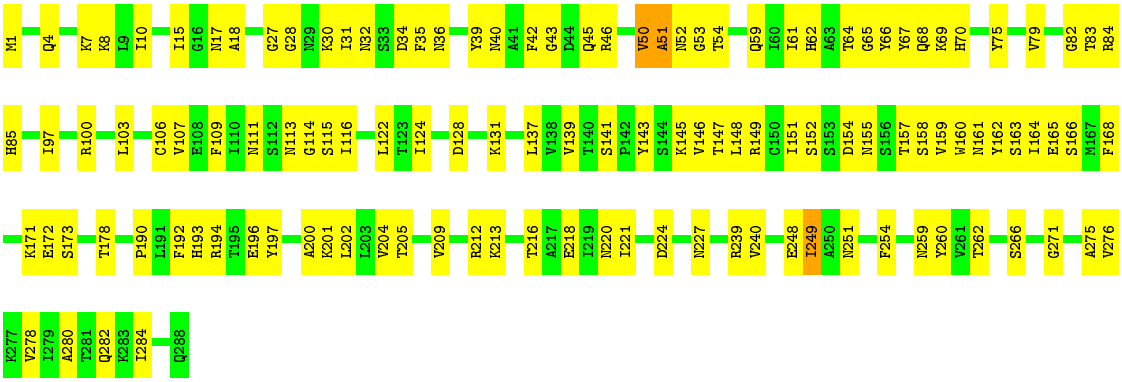


• Molecule 4: Baseplate wedge protein gp9

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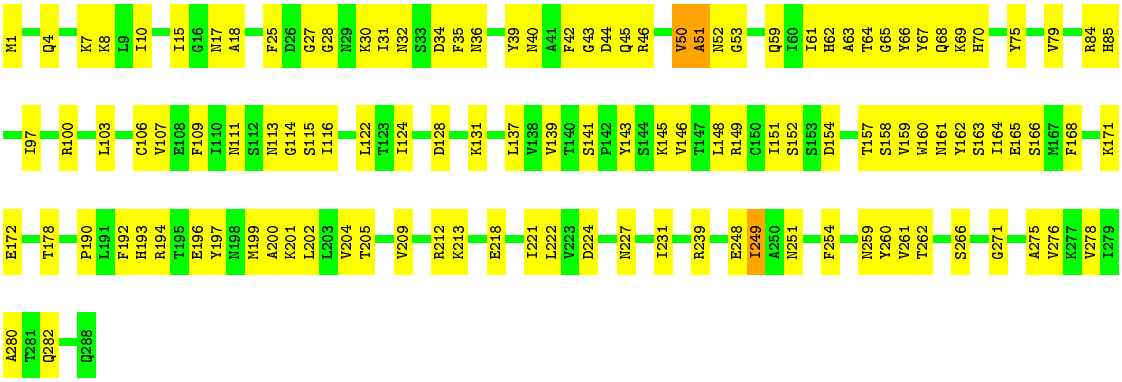
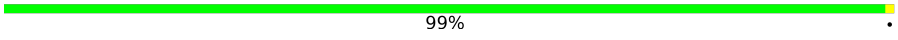
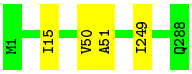



• Molecule 4: Baseplate wedge protein gp9

Chain c:




• Molecule 4: Baseplate wedge protein gp9

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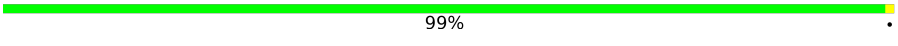
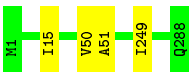
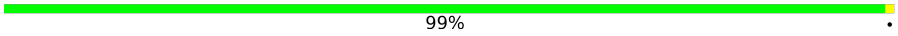
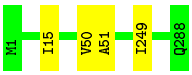





• Molecule 4: Baseplate wedge protein gp9

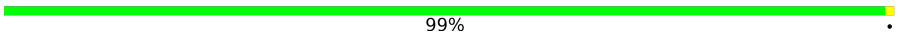
Chain e:

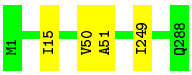



• Molecule 4: Baseplate wedge protein gp9

Chain z:




• Molecule 4: Baseplate wedge protein gp9

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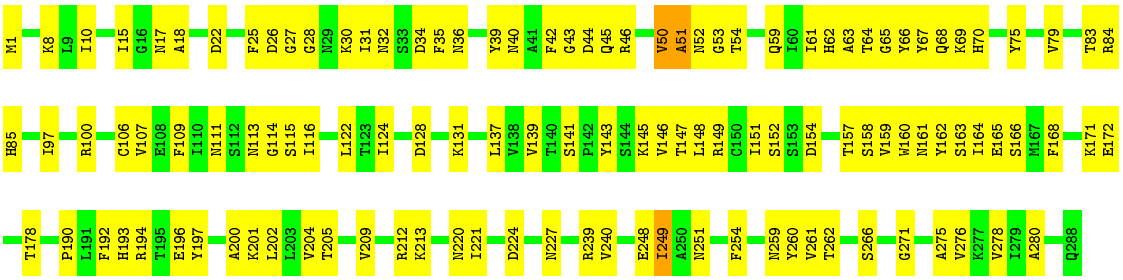
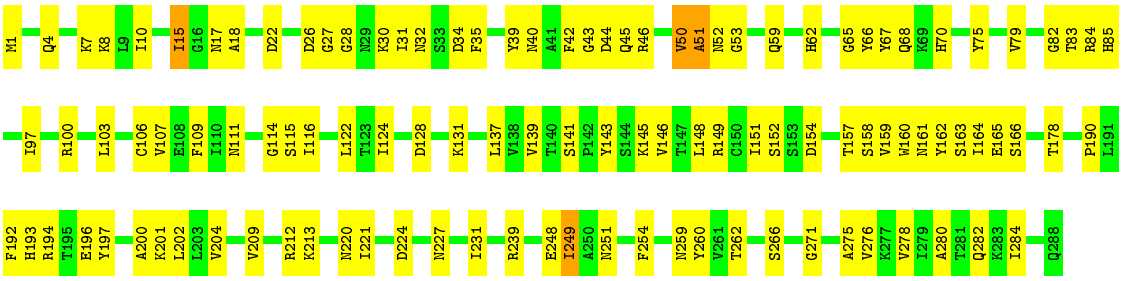



• Molecule 4: Baseplate wedge protein gp9

Chain AB:




• Molecule 4: Baseplate wedge protein gp9

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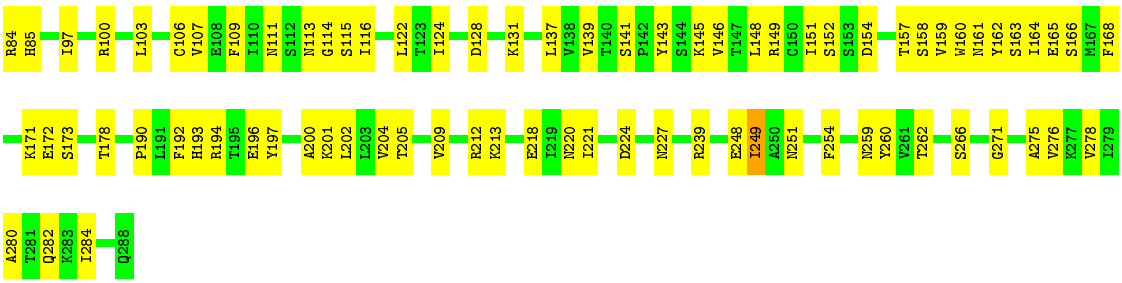
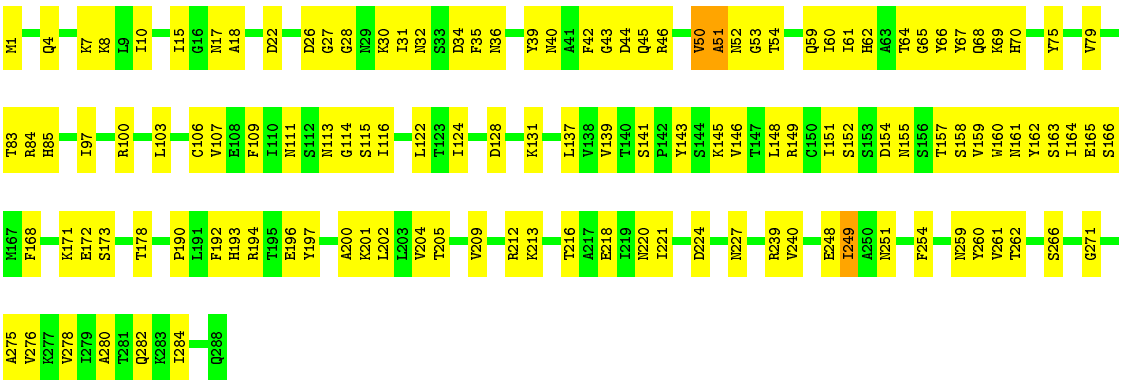


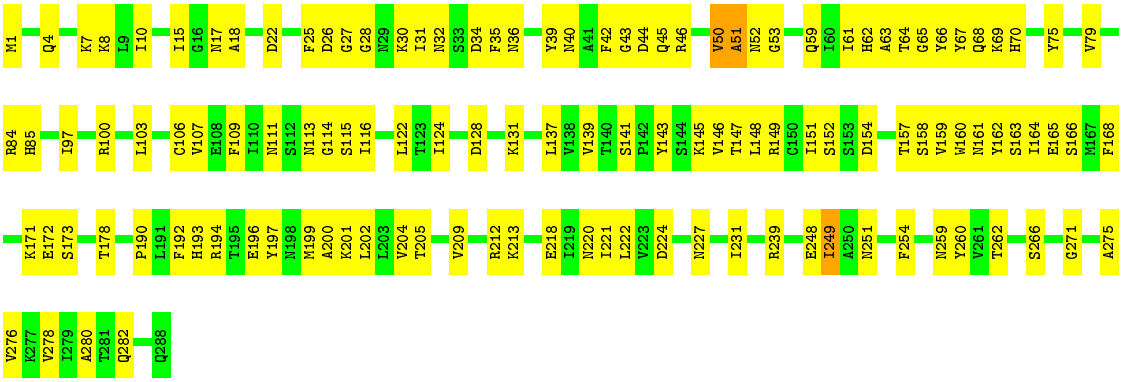

• Molecule 4: Baseplate wedge protein gp9

Chain CD: 56% 43%



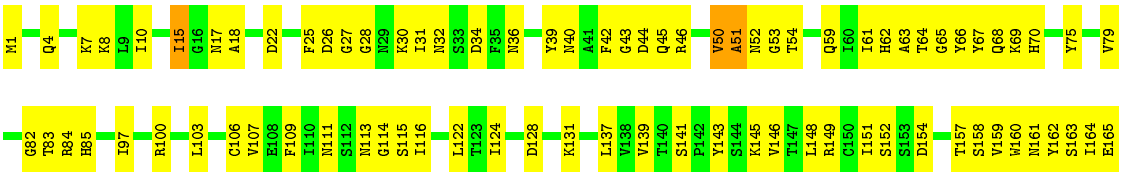

• Molecule 4: Baseplate wedge protein gp9

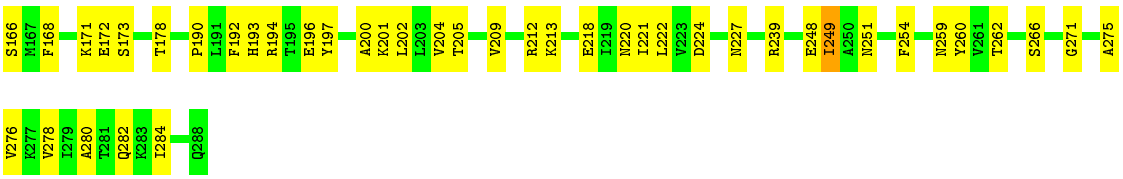
Chain CE: 57% 42%




• Molecule 4: Baseplate wedge protein gp9

Chain EF: 57% 42%






• Molecule 4: Baseplate wedge protein gp9

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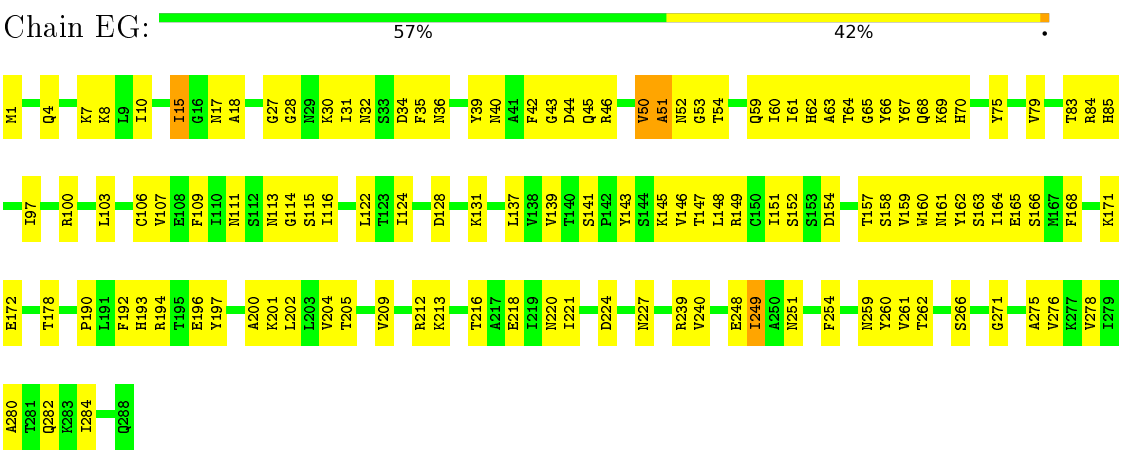


• Molecule 4: Baseplate wedge protein gp9

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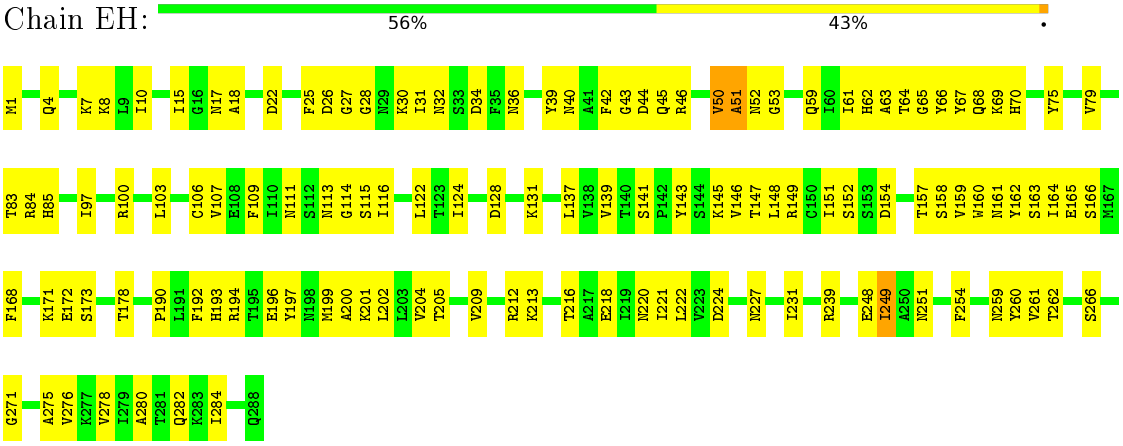
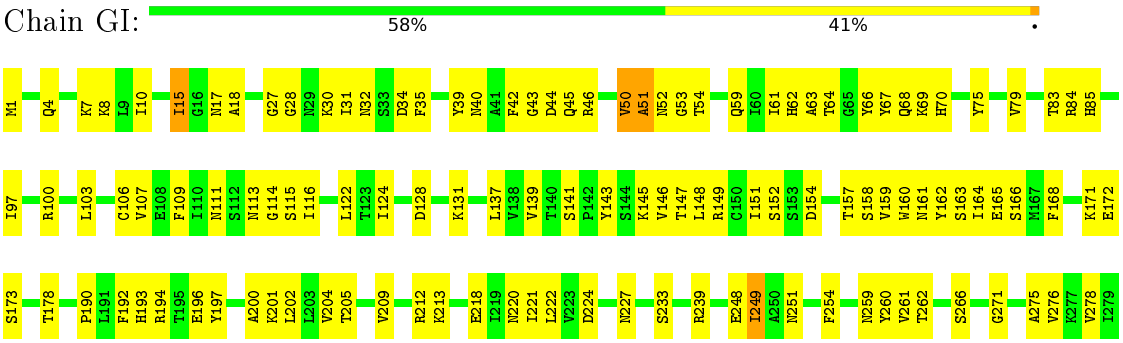
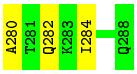



• Molecule 4: Baseplate wedge protein gp9

Chain GI:






• Molecule 4: Baseplate wedge protein gp9

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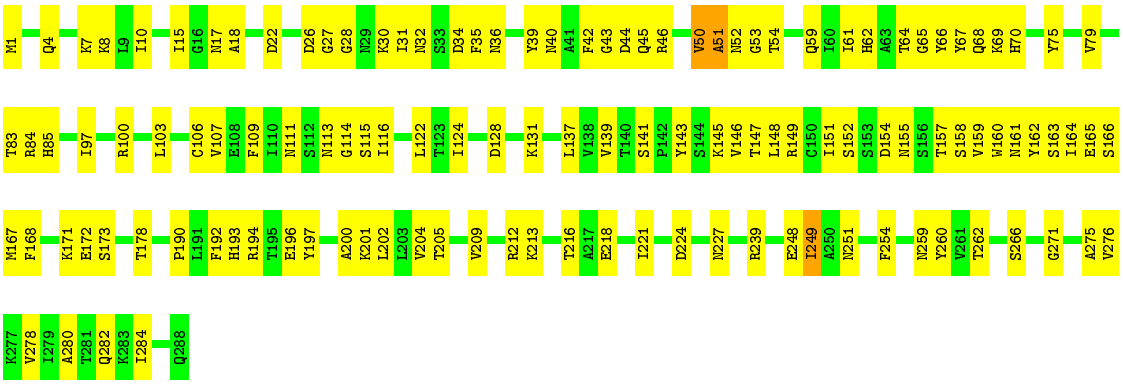


• Molecule 4: Baseplate wedge protein gp9

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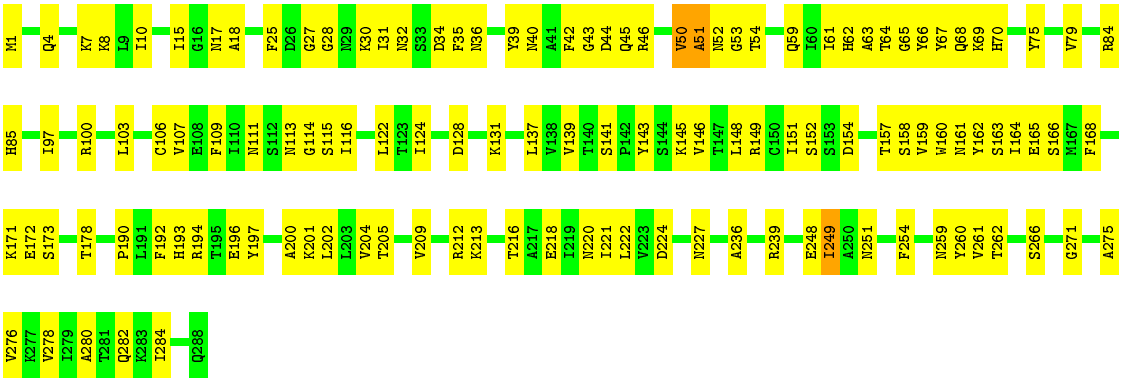


• Molecule 5: Baseplate wedge protein gp10

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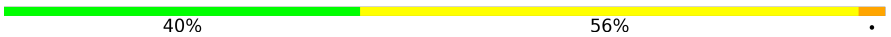
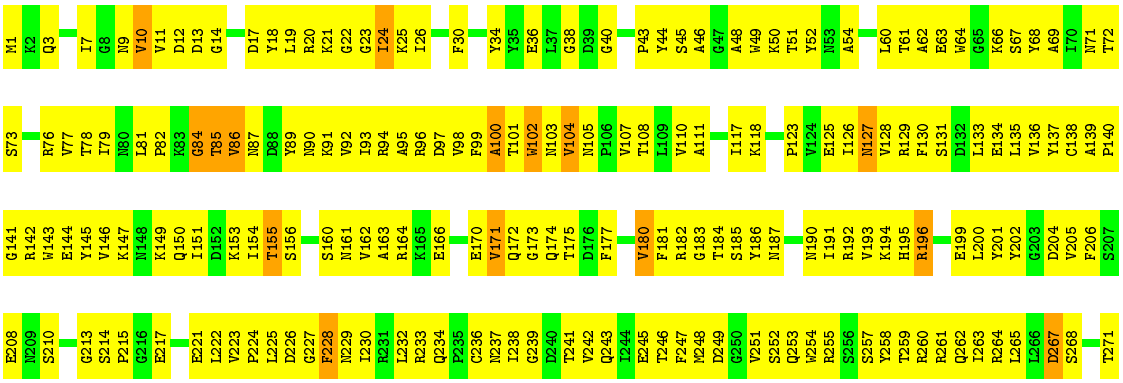
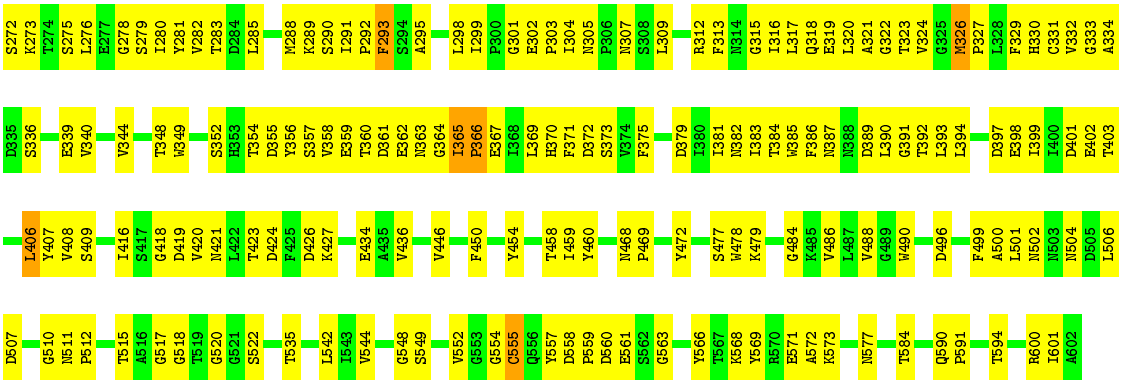
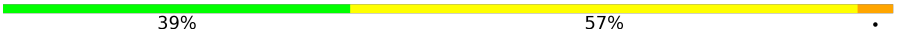


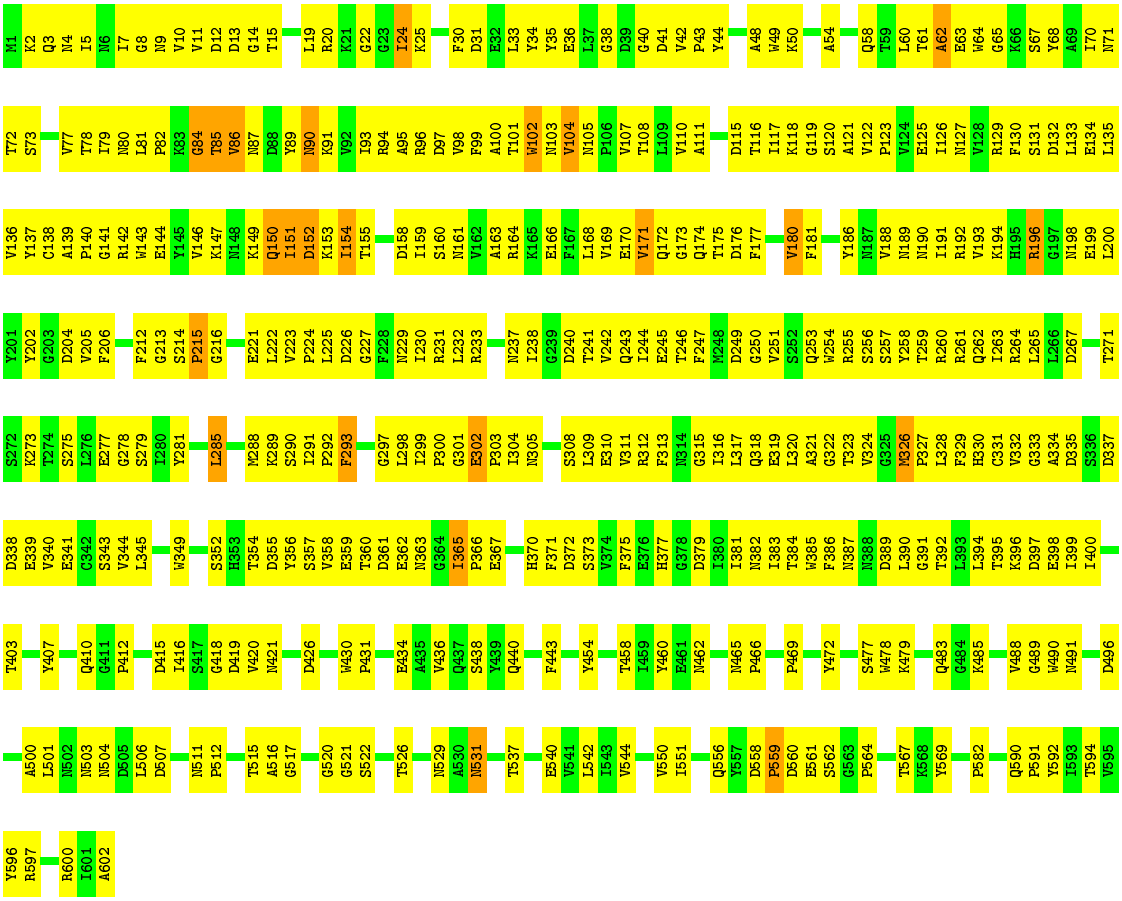





• Molecule 5: Baseplate wedge protein gp10

Chain J:



• Molecule 5: Baseplate wedge protein gp10

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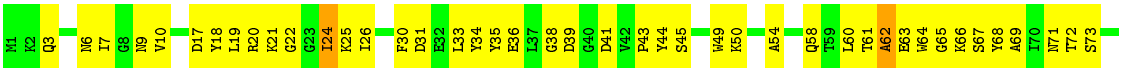

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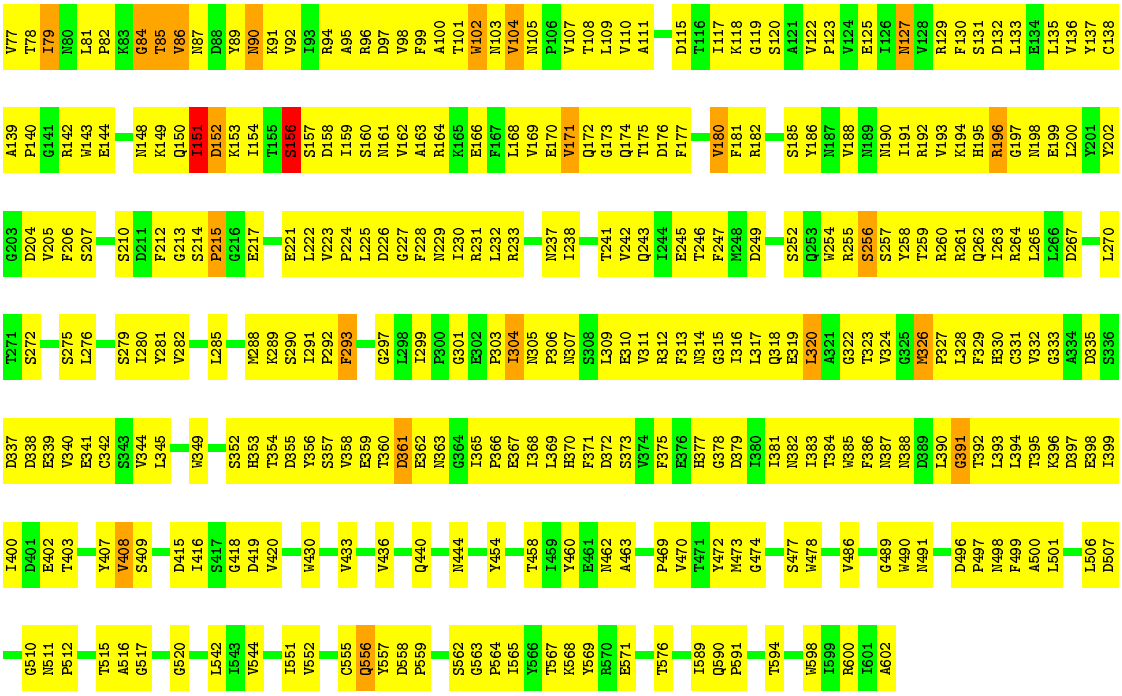
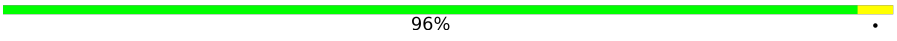


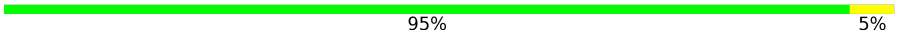

- Molecule 5: Baseplate wedge protein gp10

Chain f:



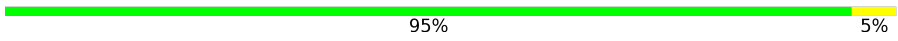
- Molecule 5: Baseplate wedge protein gp10

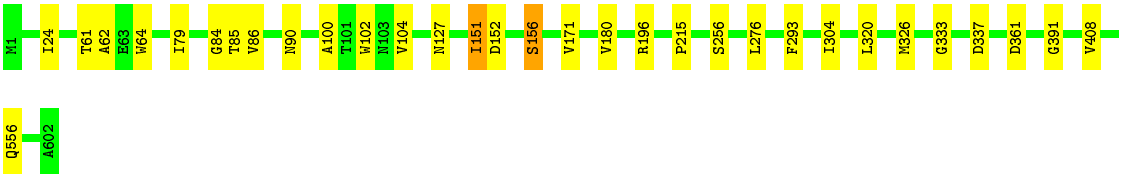
Chain g:



- Molecule 5: Baseplate wedge protein gp10

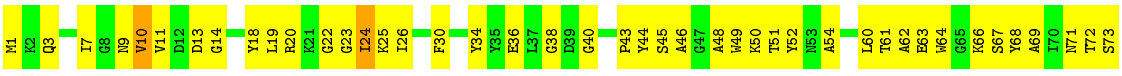
Chain h:

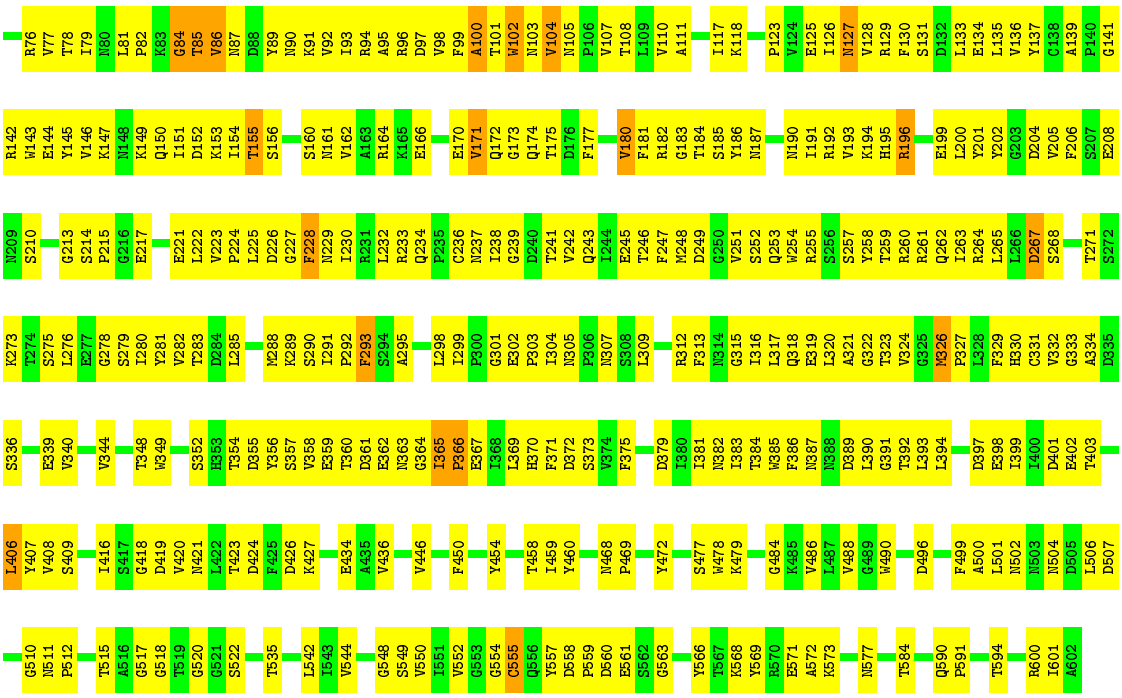



- Molecule 5: Baseplate wedge protein gp10

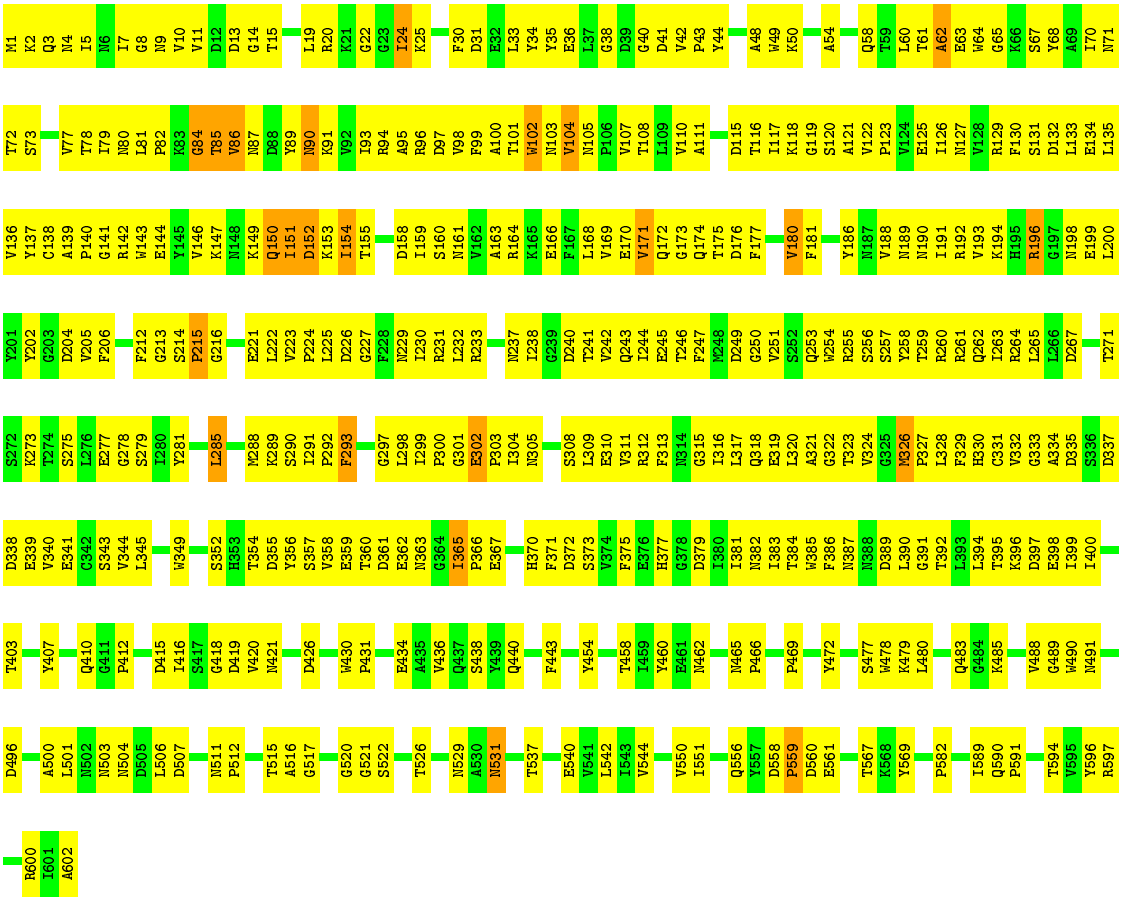
Chain AC:





• Molecule 5: Baseplate wedge protein gp10

Chain AD:



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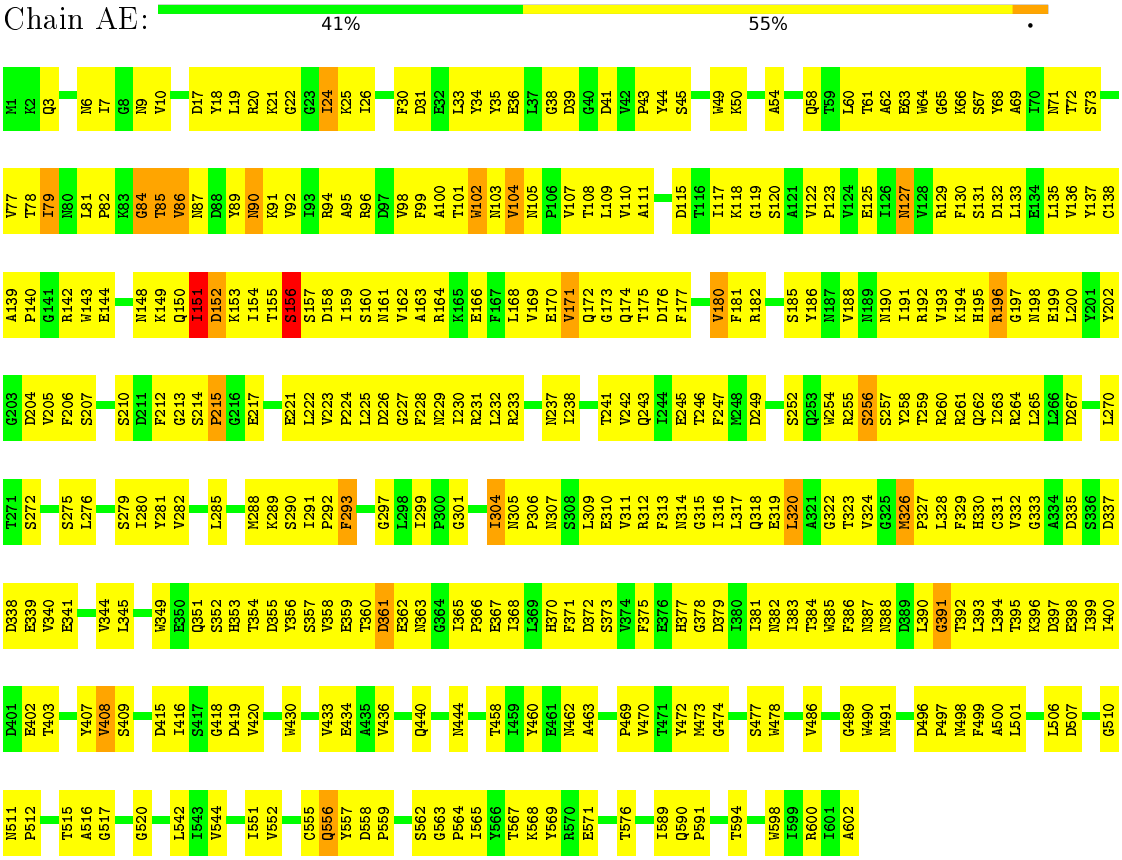
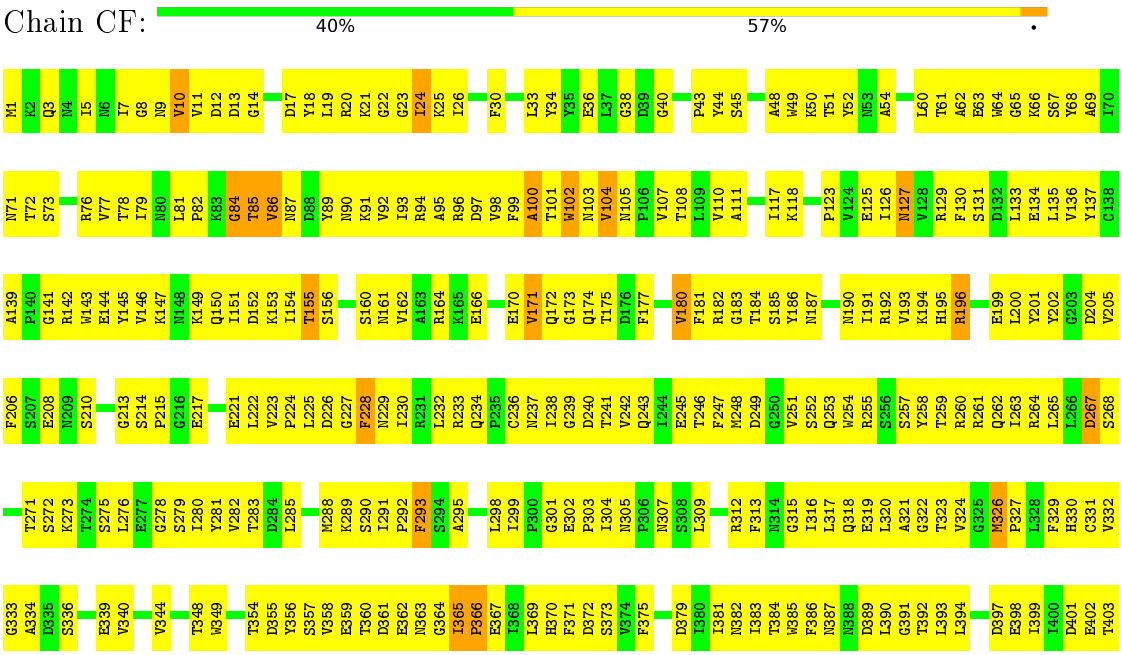
• Molecule 5: Baseplate wedge protein gp10

Chain AE:

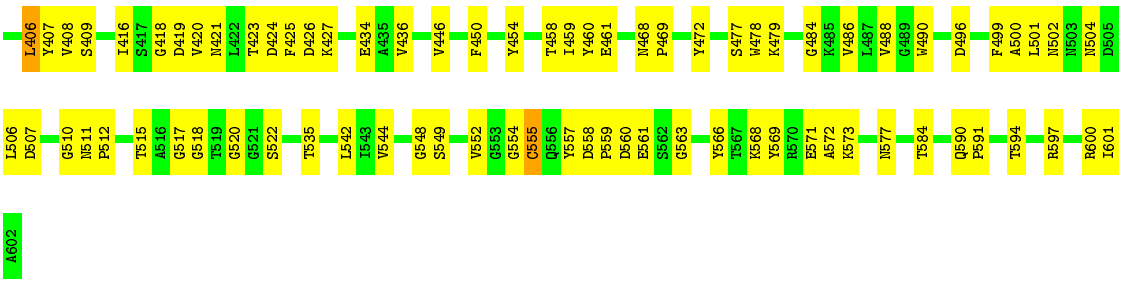



• Molecule 5: Baseplate wedge protein gp10

Chain CF:




WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

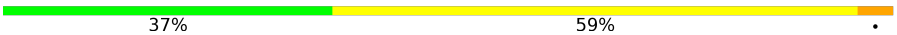


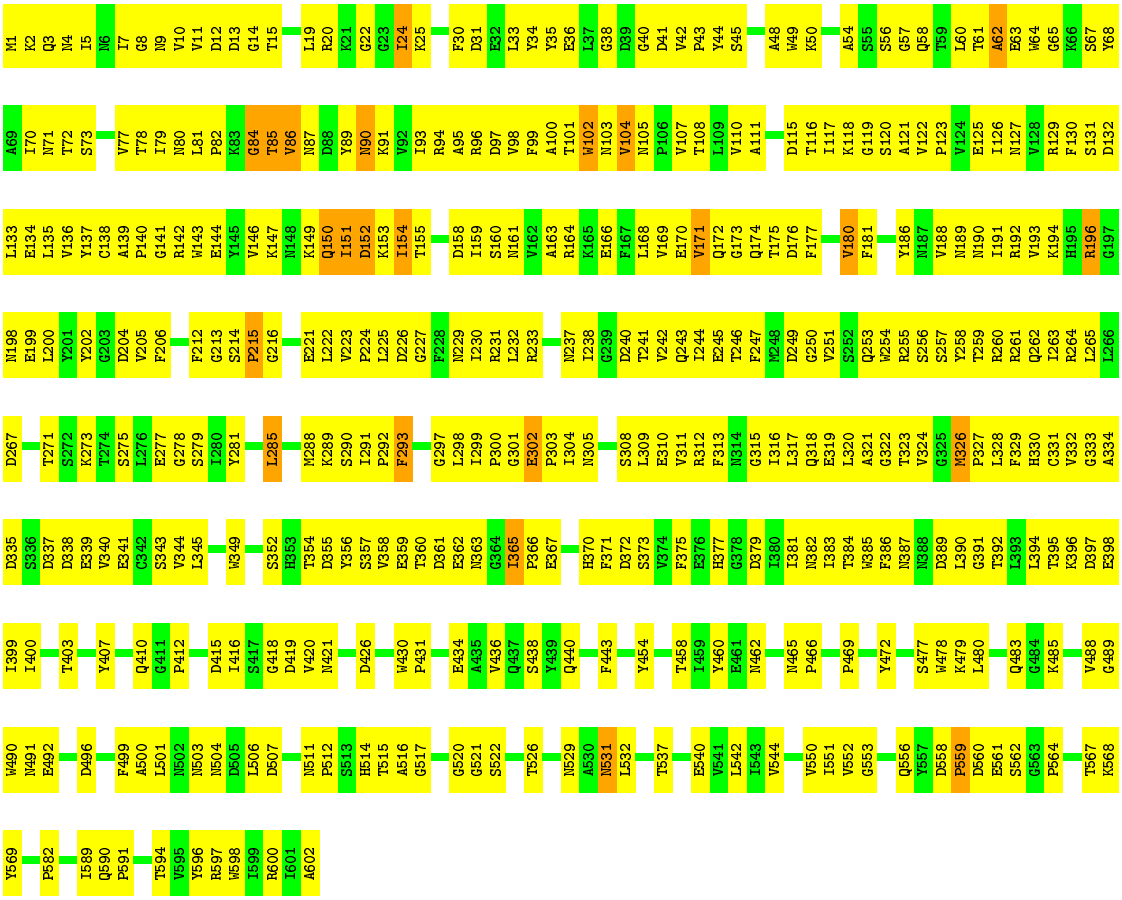




• Molecule 5: Baseplate wedge protein gp10

Chain CG:

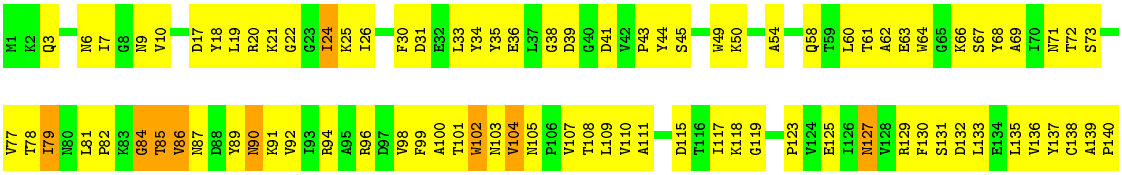


• Molecule 5: Baseplate wedge protein gp10

Chain CH:



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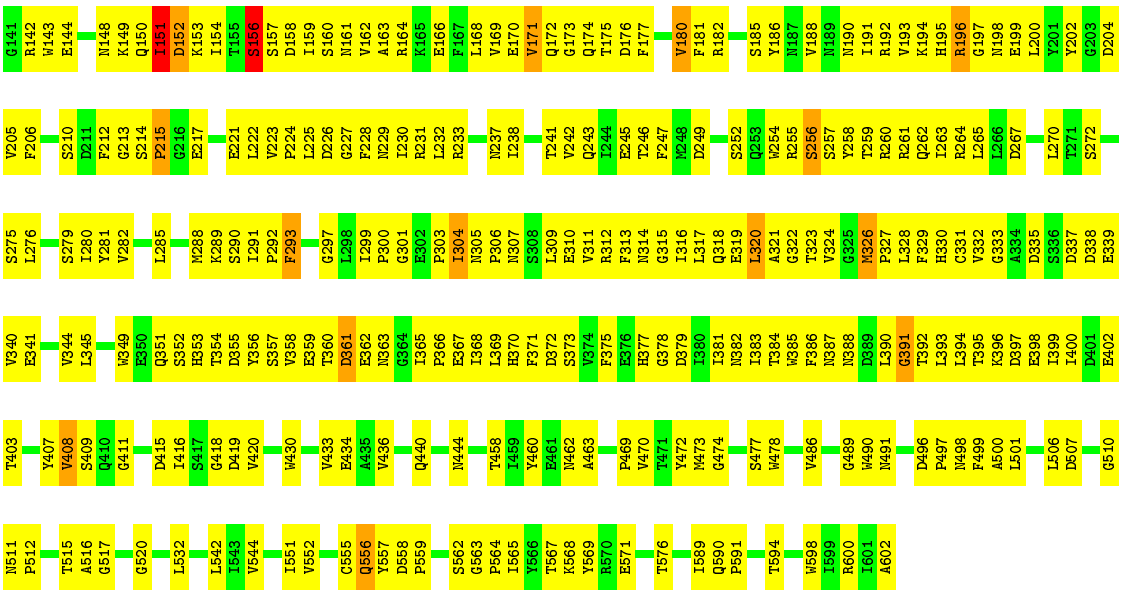

• Molecule 5: Baseplate wedge protein gp10

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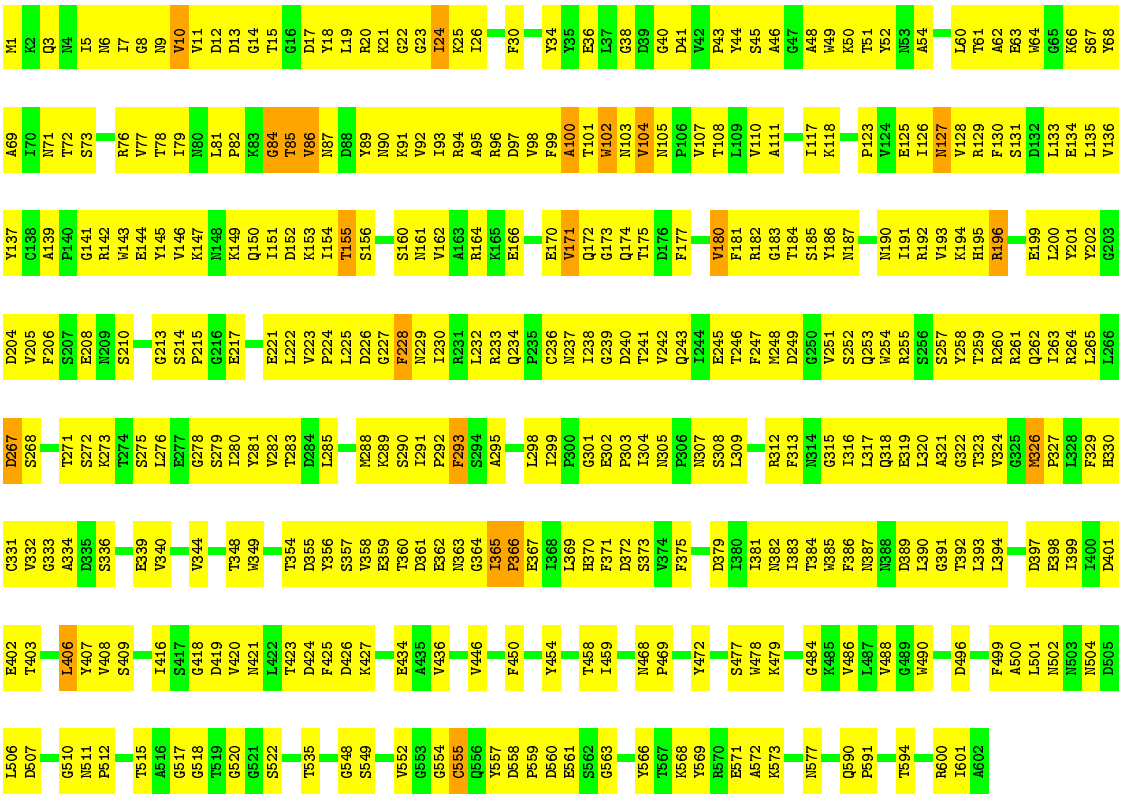
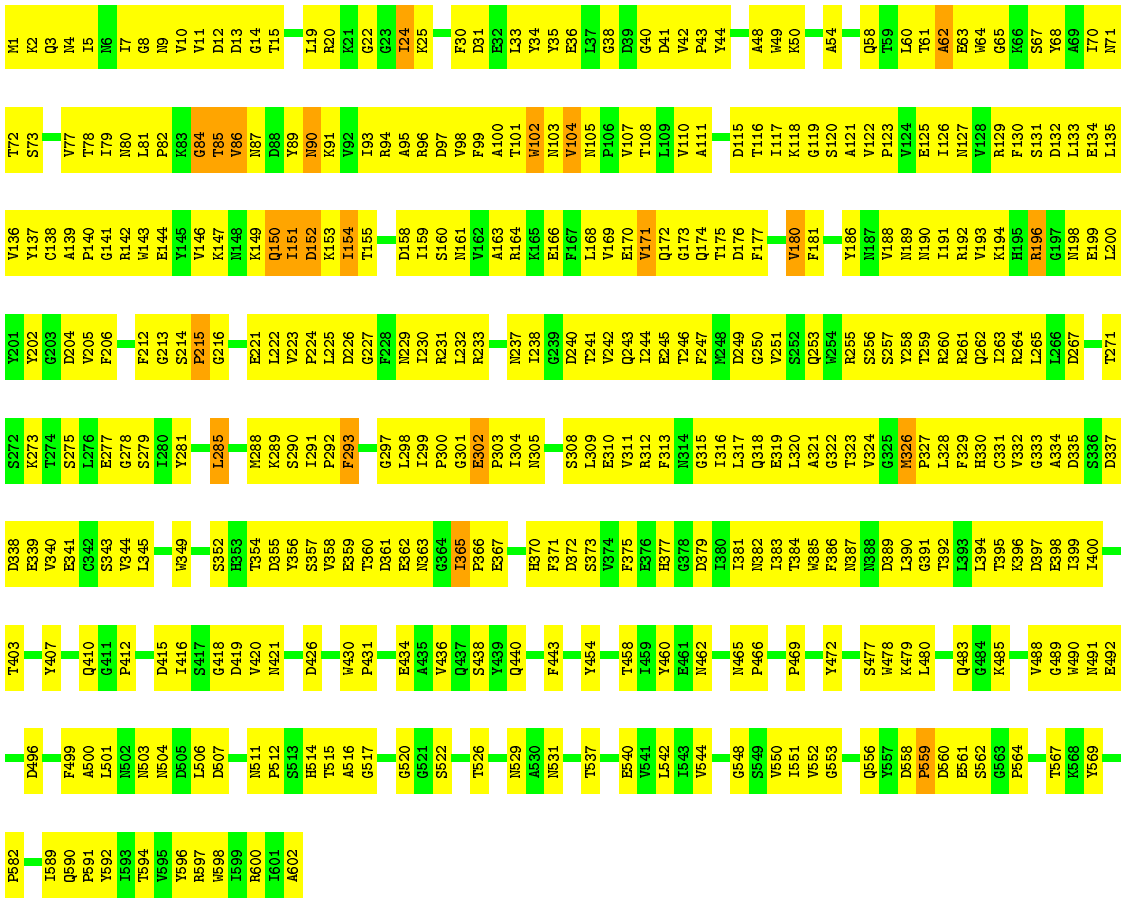


• Molecule 5: Baseplate wedge protein gp10

Chain EJ:

WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



• Molecule 5: Baseplate wedge protein gp10

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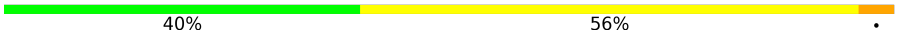


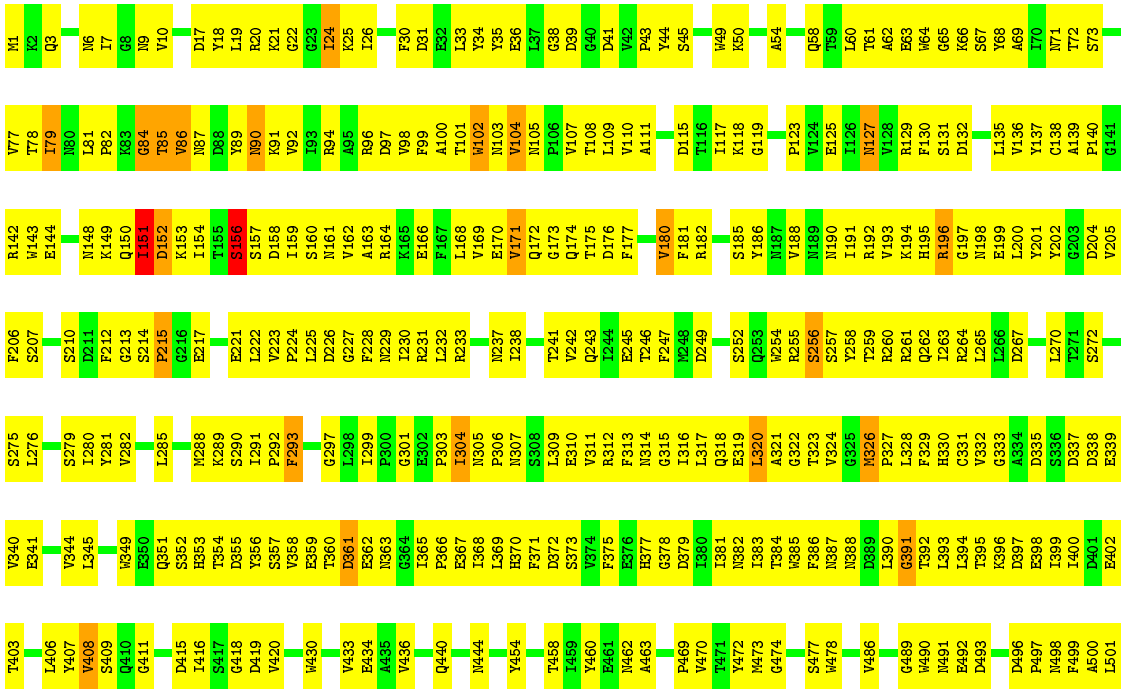

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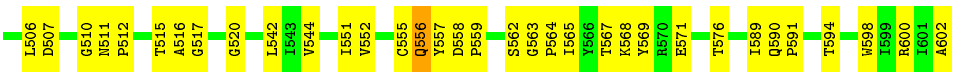


• Molecule 5: Baseplate wedge protein gp10

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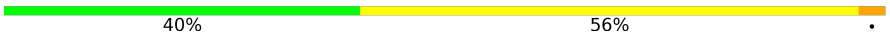


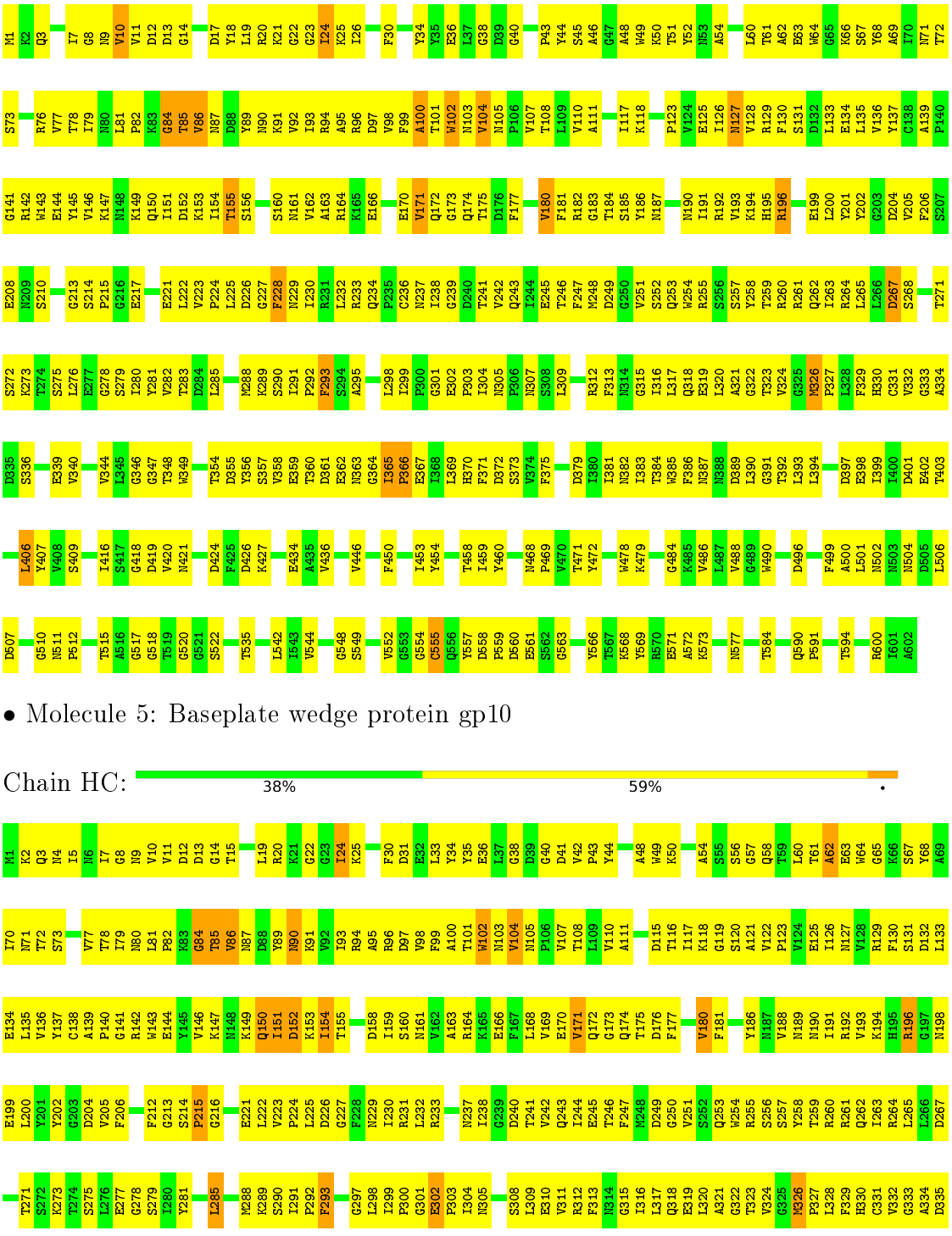

• Molecule 5: Baseplate wedge protein gp10

Chain HC:






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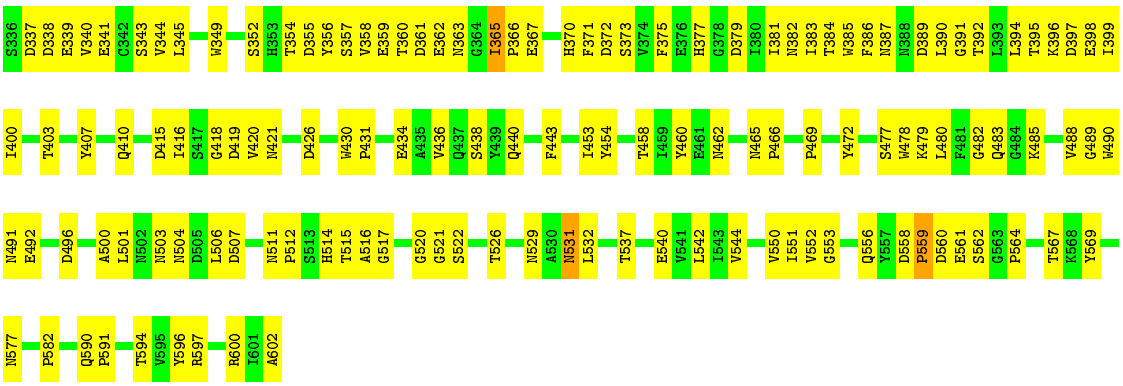

• Molecule 5: Baseplate wedge protein gp10

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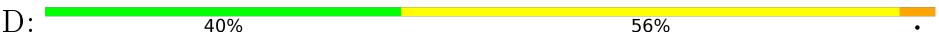


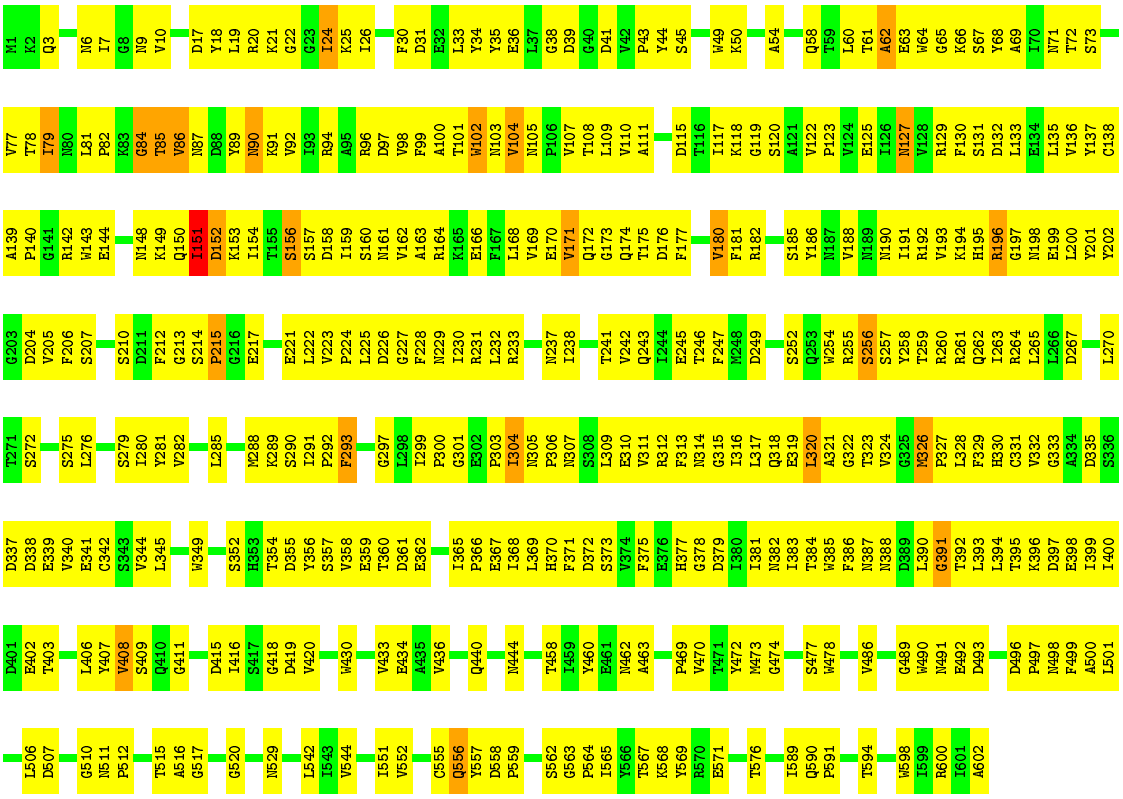

• Molecule 6: Baseplate wedge protein gp11

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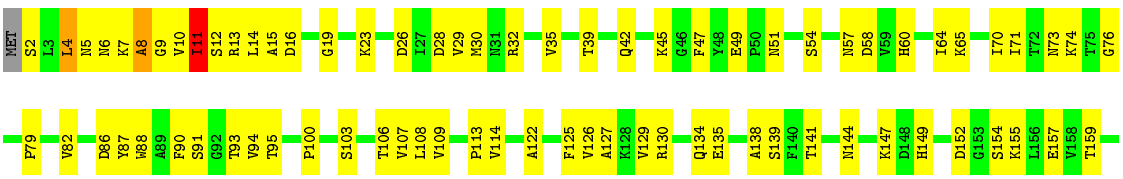

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• Molecule 6: Baseplate wedge protein gp11

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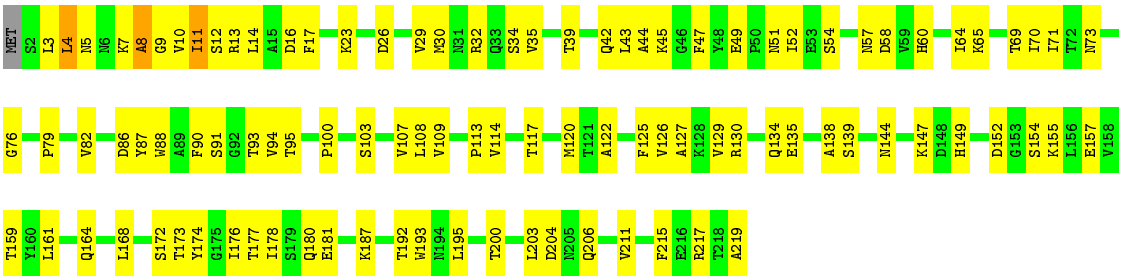


• Molecule 6: Baseplate wedge protein gp11

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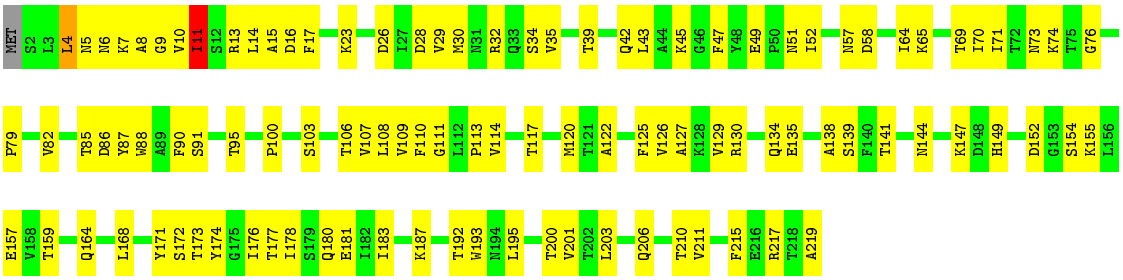
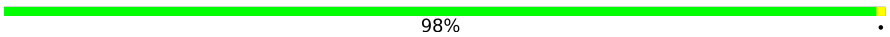
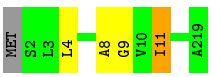



• Molecule 6: Baseplate wedge protein gp11

Chain i:




• Molecule 6: Baseplate wedge protein gp11

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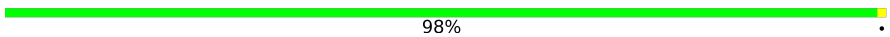


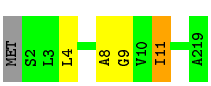


• Molecule 6: Baseplate wedge protein gp11

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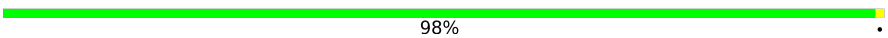


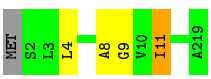


• Molecule 6: Baseplate wedge protein gp11

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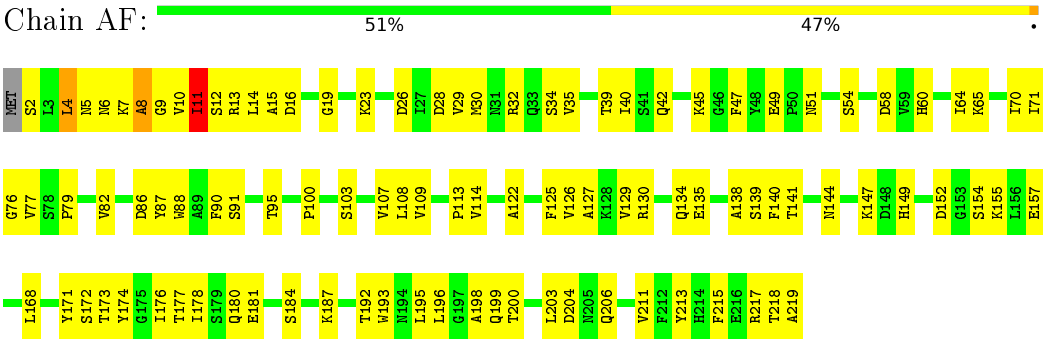


- Molecule 6: Baseplate wedge protein gp11

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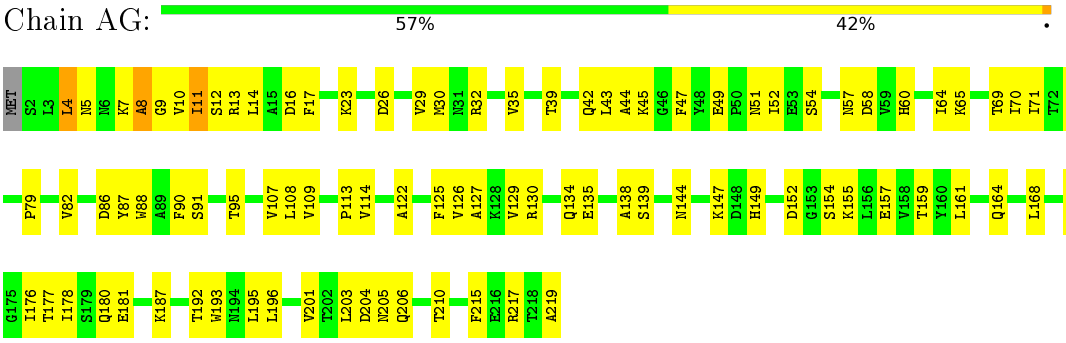


- Molecule 6: Baseplate wedge protein gp11

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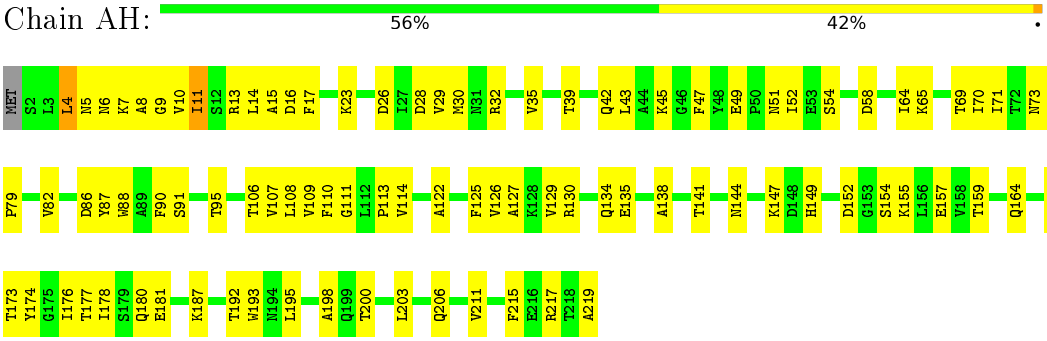


- Molecule 6: Baseplate wedge protein gp11

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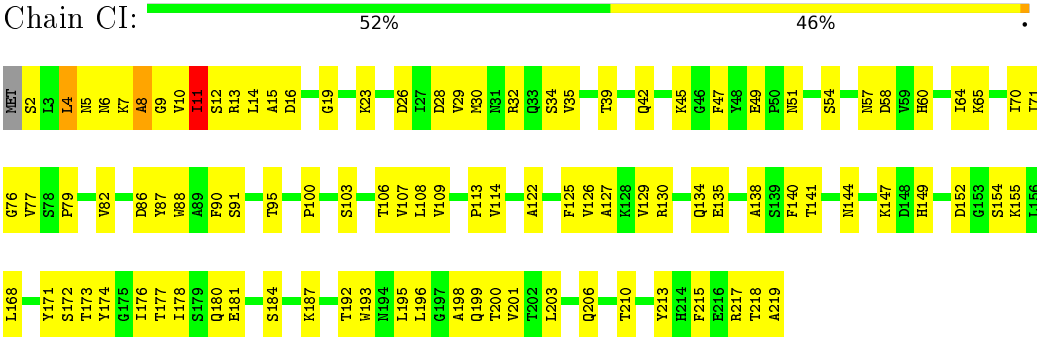


- Molecule 6: Baseplate wedge protein gp11

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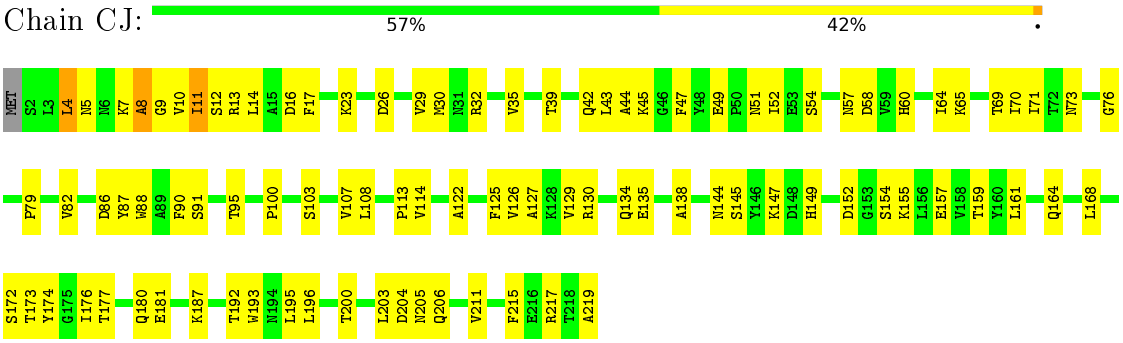


- Molecule 6: Baseplate wedge protein gp11

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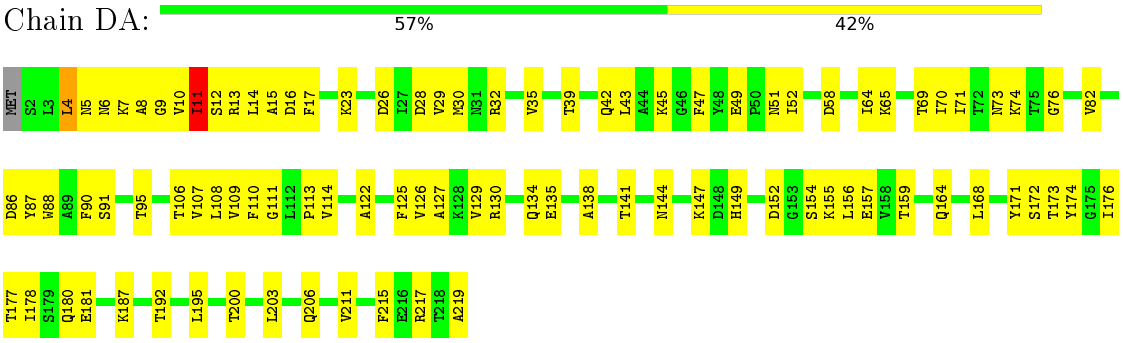


- Molecule 6: Baseplate wedge protein gp11

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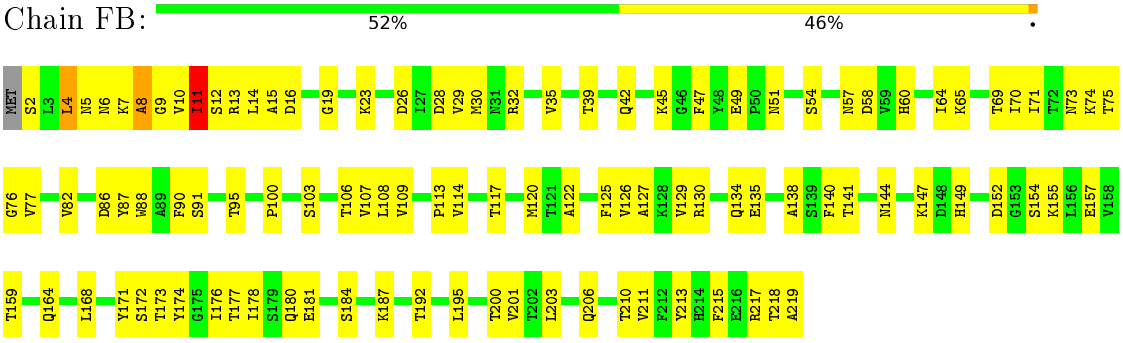


- Molecule 6: Baseplate wedge protein gp11

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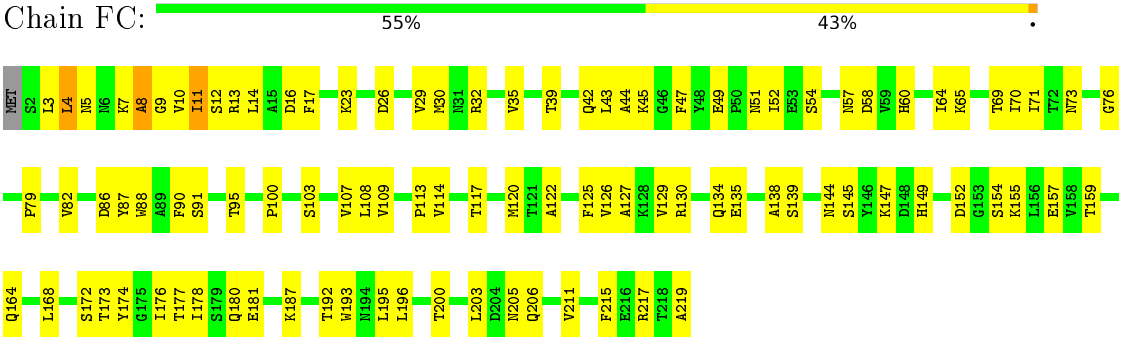


- Molecule 6: Baseplate wedge protein gp11

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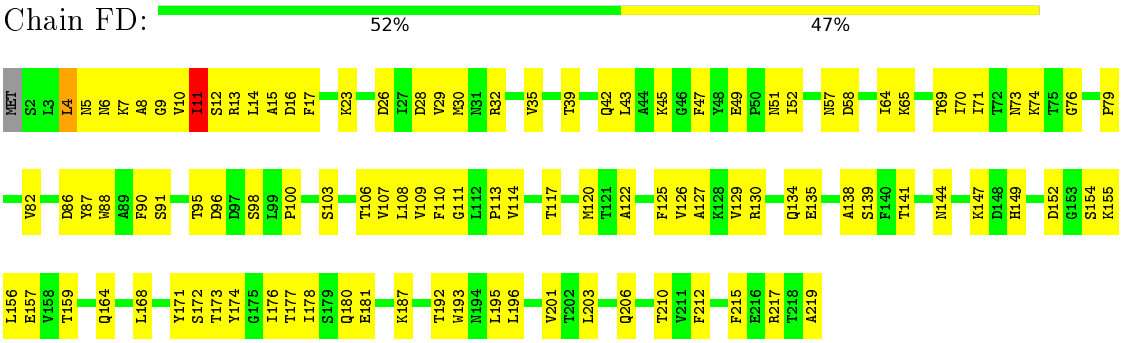


• Molecule 6: Baseplate wedge protein gp11

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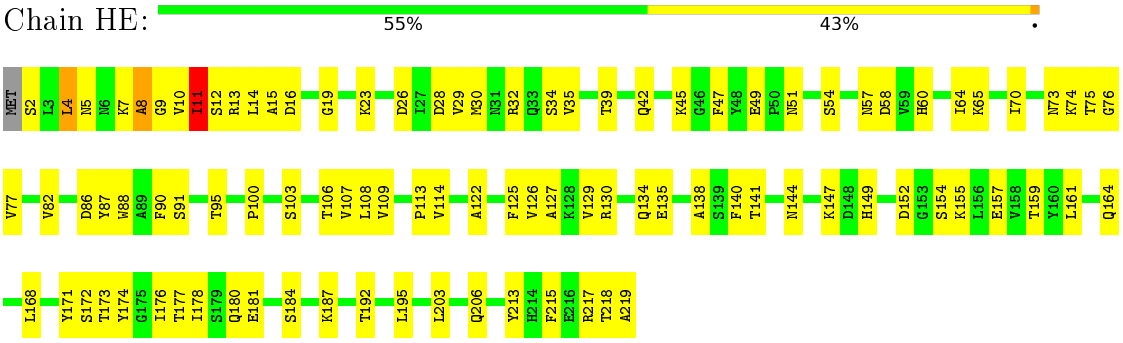
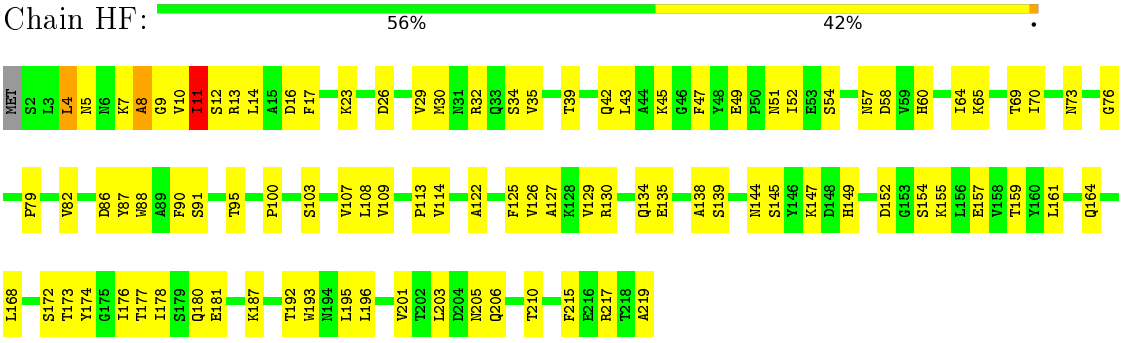



• Molecule 6: Baseplate wedge protein gp11

Chain HF:




• Molecule 6: Baseplate wedge protein gp11

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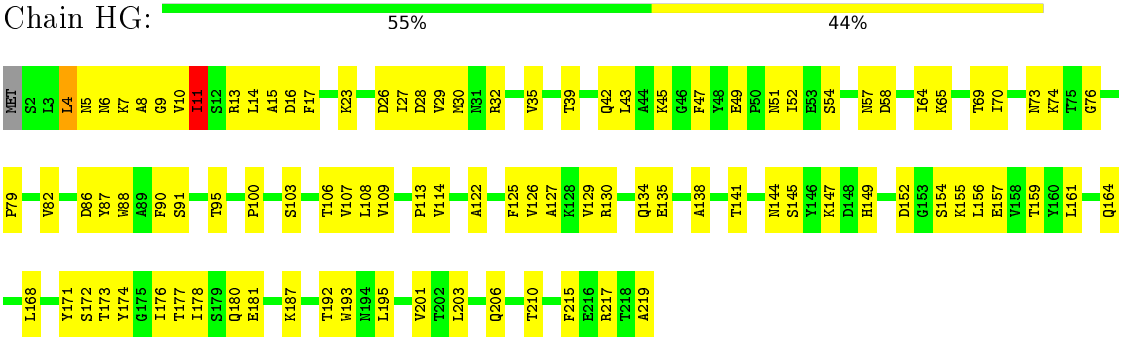


• Molecule 7: Short tail fiber protein gp12

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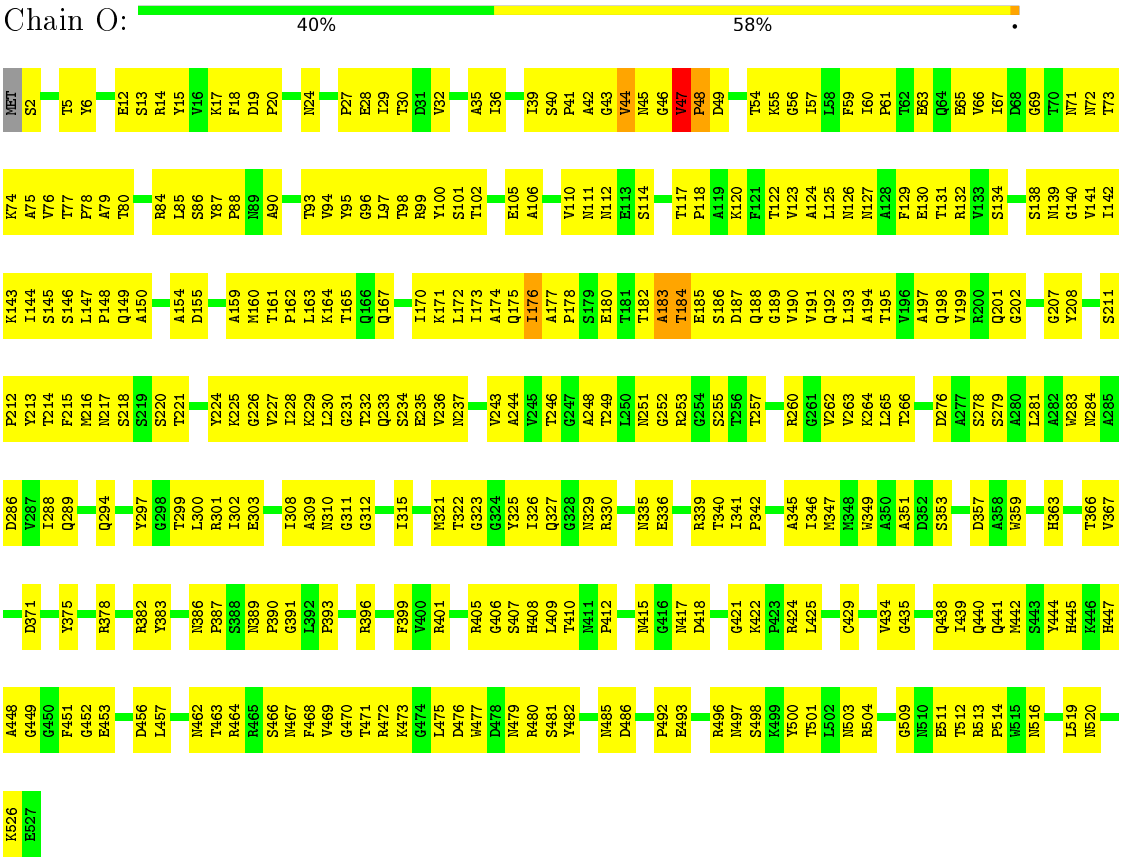
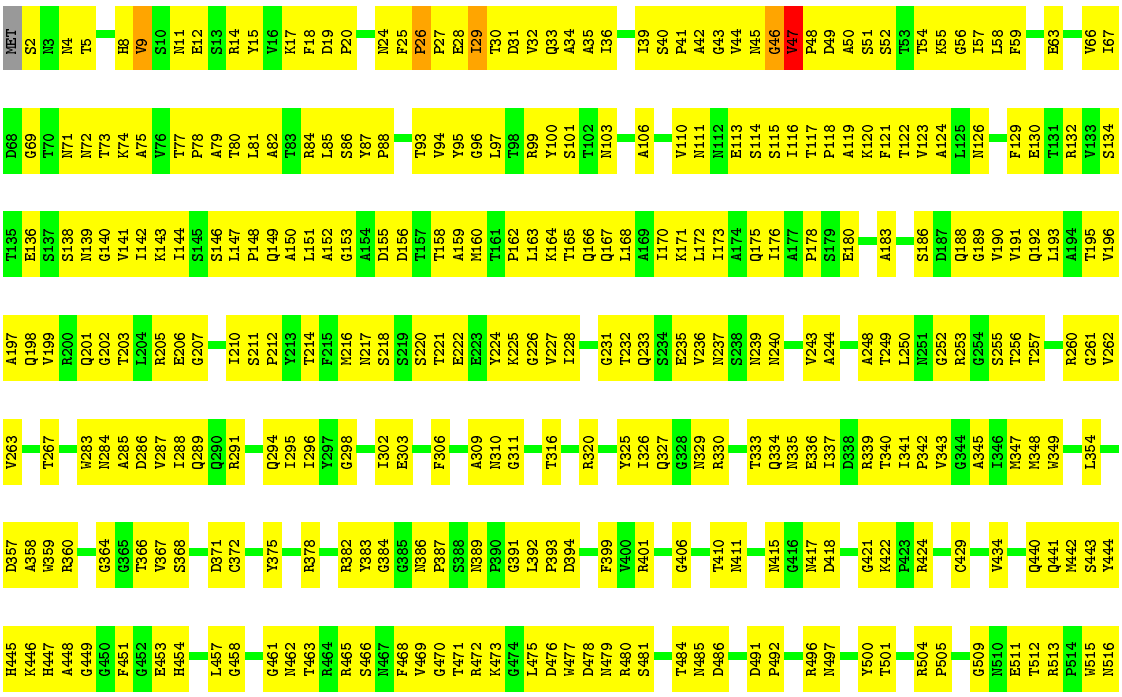



• Molecule 7: Short tail fiber protein gp12

Chain P:

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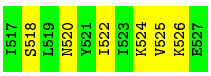
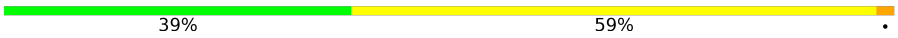
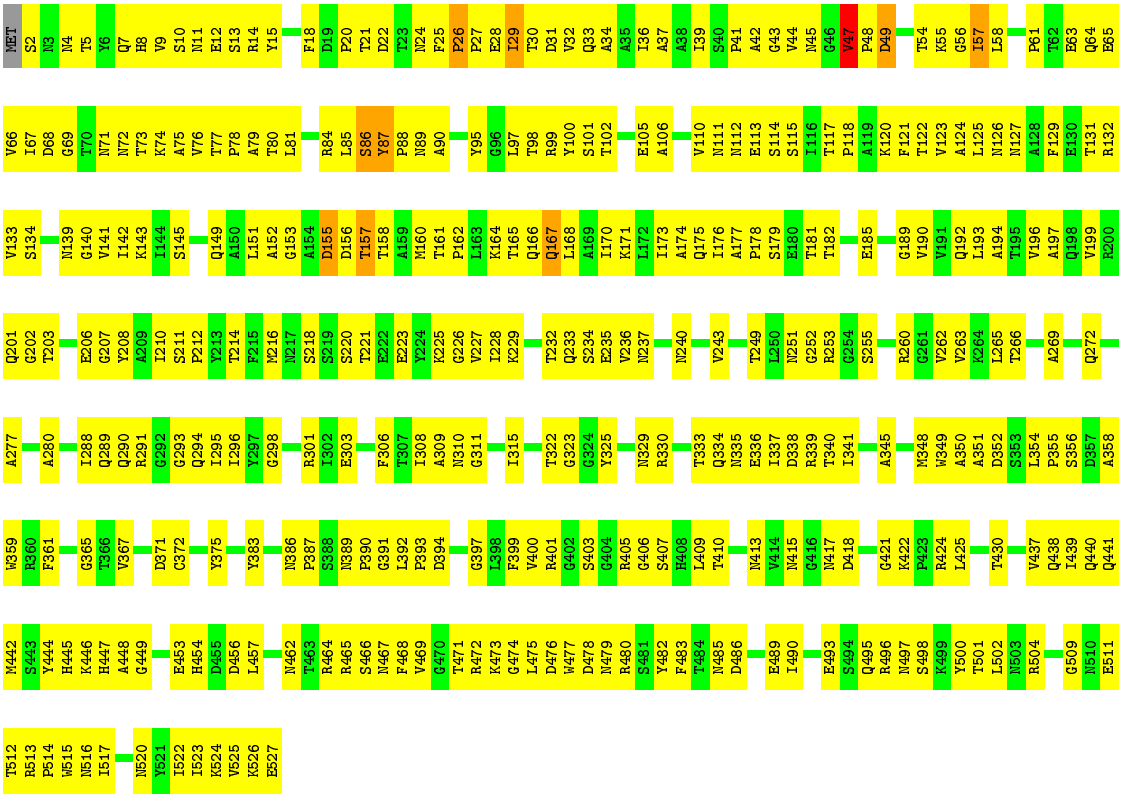



• Molecule 7: Short tail fiber protein gp12

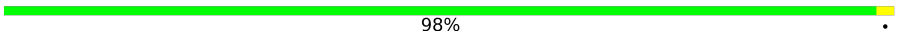
Chain Q:

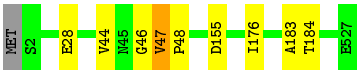



• Molecule 7: Short tail fiber protein gp12

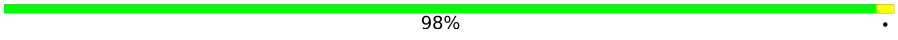
Chain l:

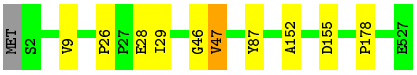



• Molecule 7: Short tail fiber protein gp12

Chain m:




• Molecule 7: Short tail fiber protein gp12

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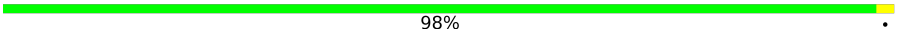


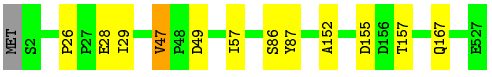

• Molecule 7: Short tail fiber protein gp12

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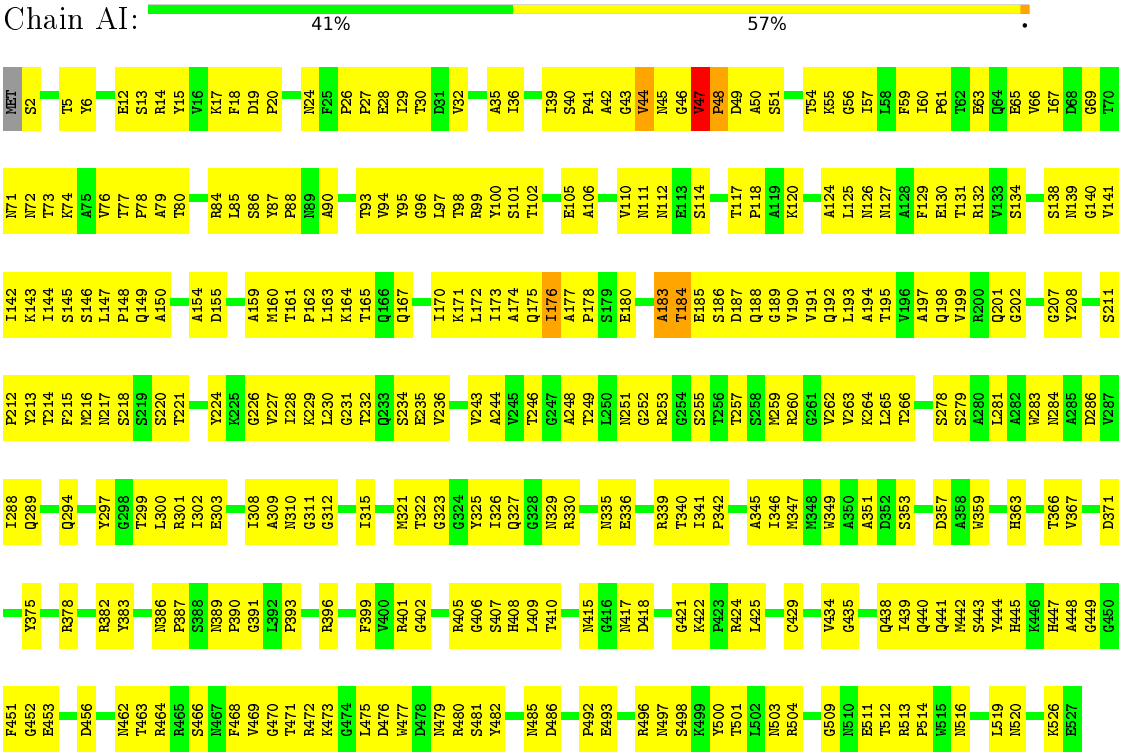


• Molecule 7: Short tail fiber protein gp12

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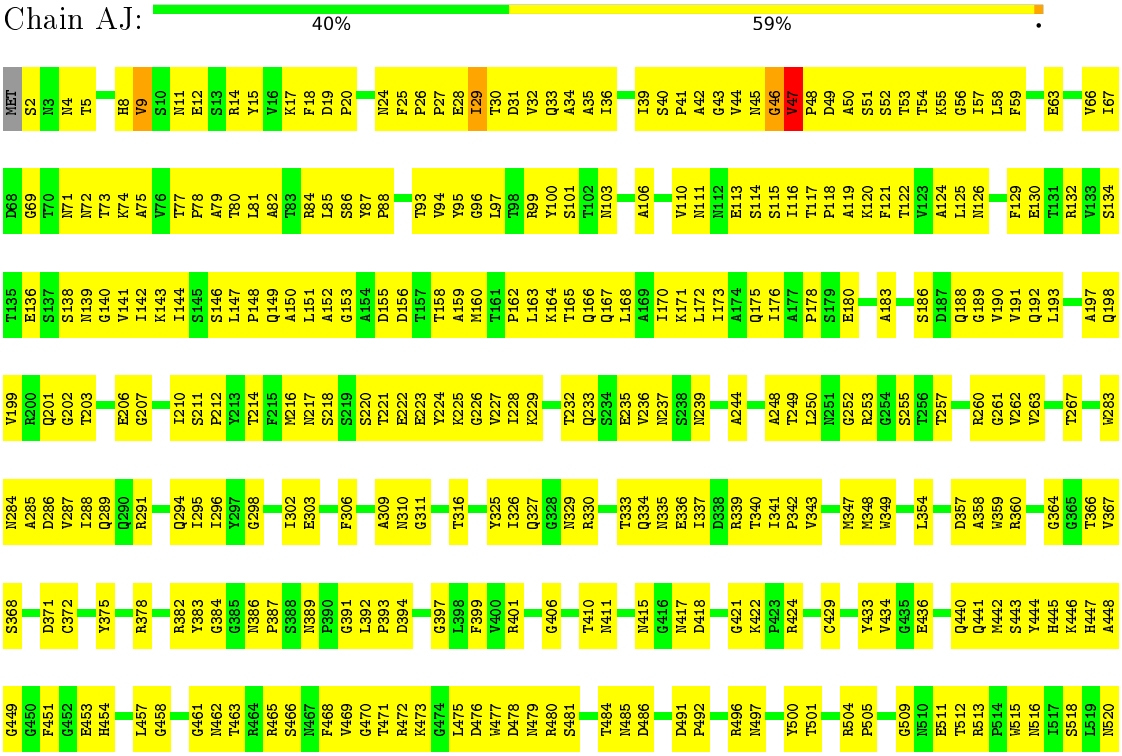
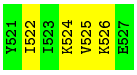



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM




• Molecule 7: Short tail fiber protein gp12

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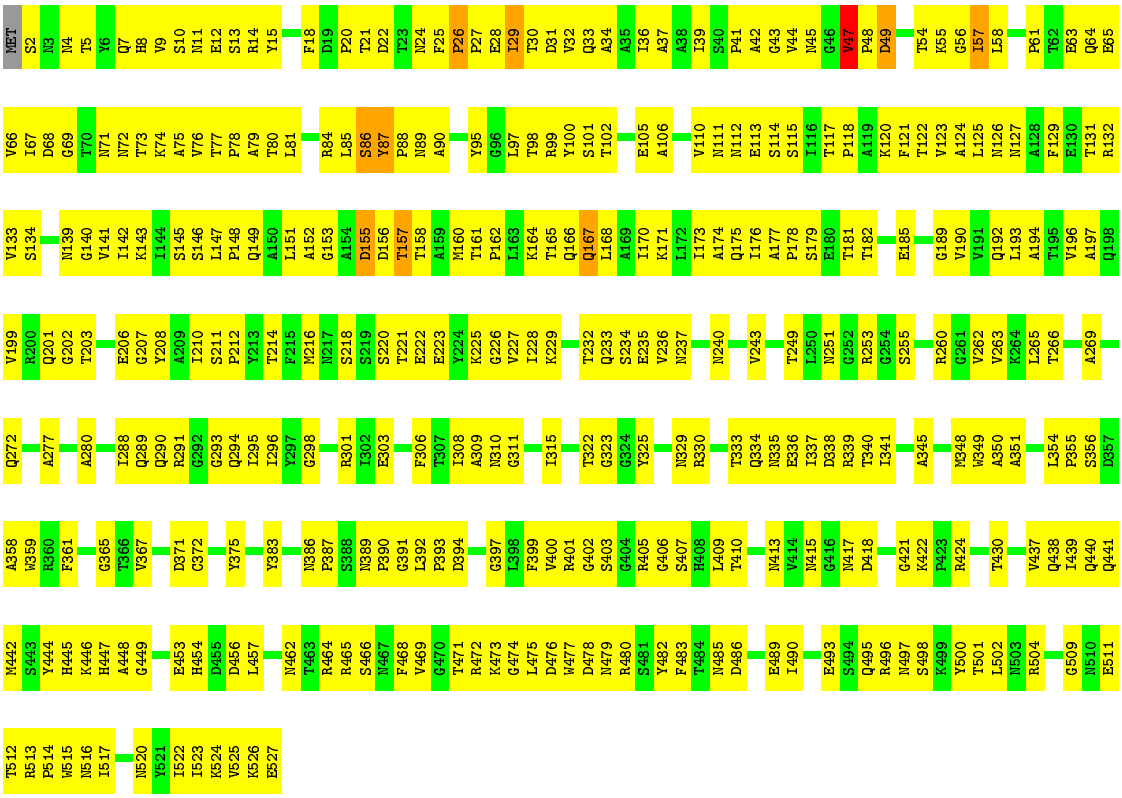


• Molecule 7: Short tail fiber protein gp12

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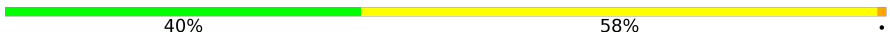


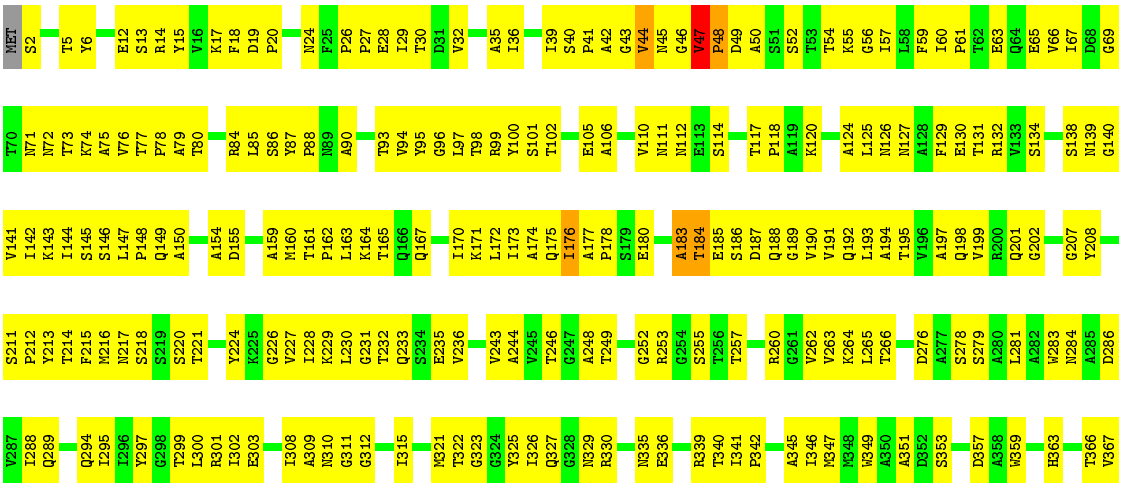

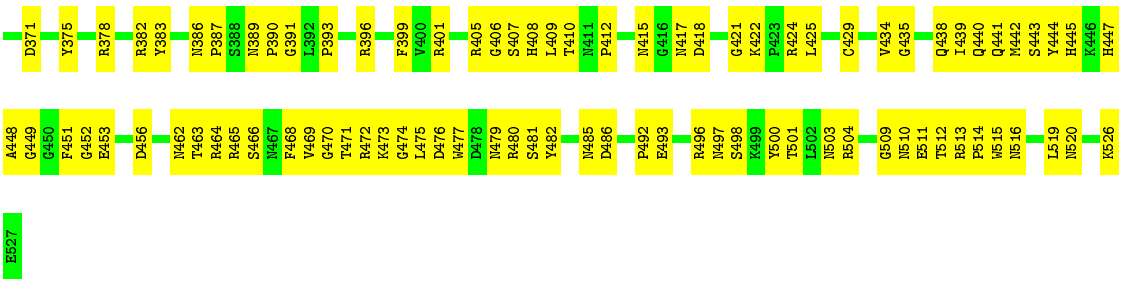


• Molecule 7: Short tail fiber protein gp12

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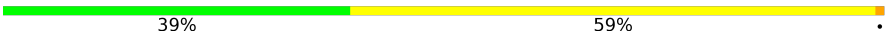


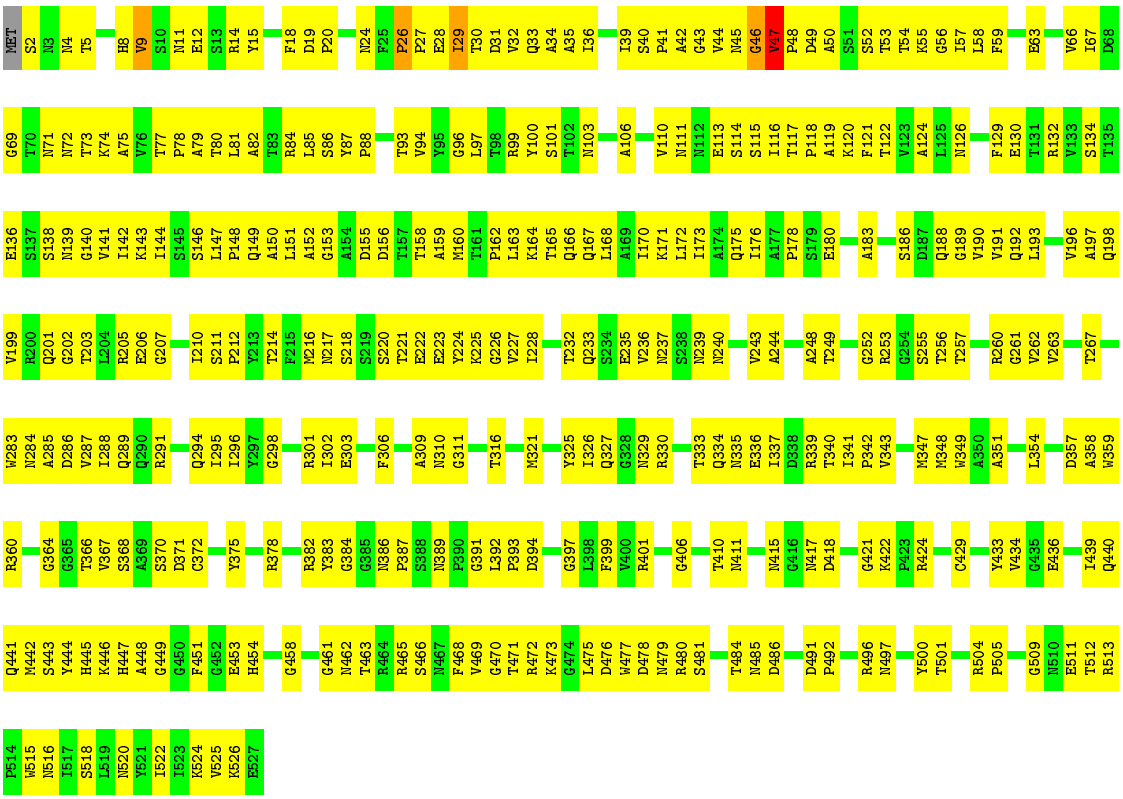


• Molecule 7: Short tail fiber protein gp12

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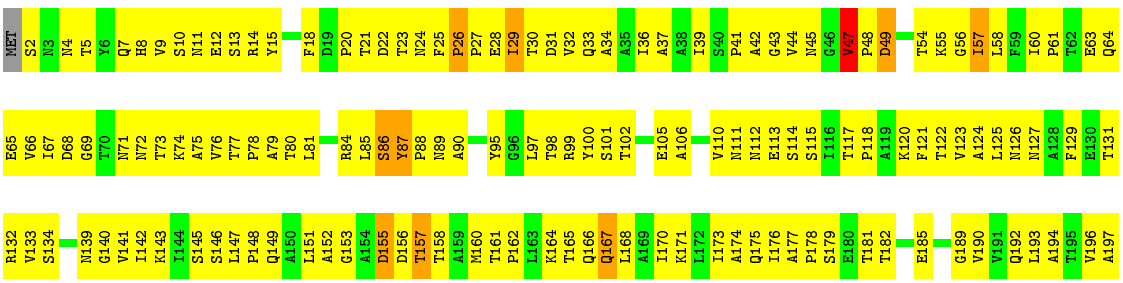
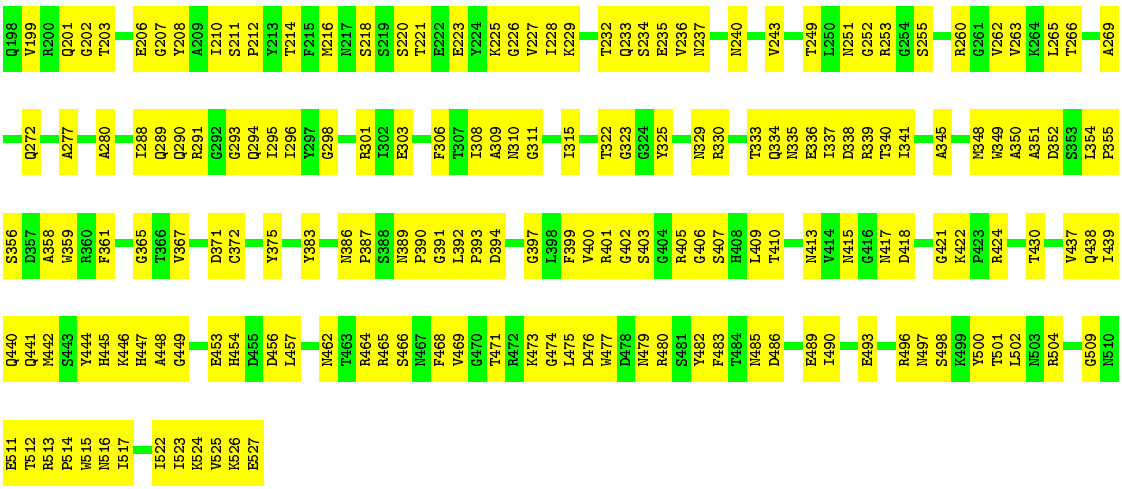



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM




- Molecule 7: Short tail fiber protein gp12

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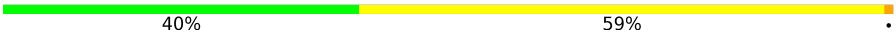


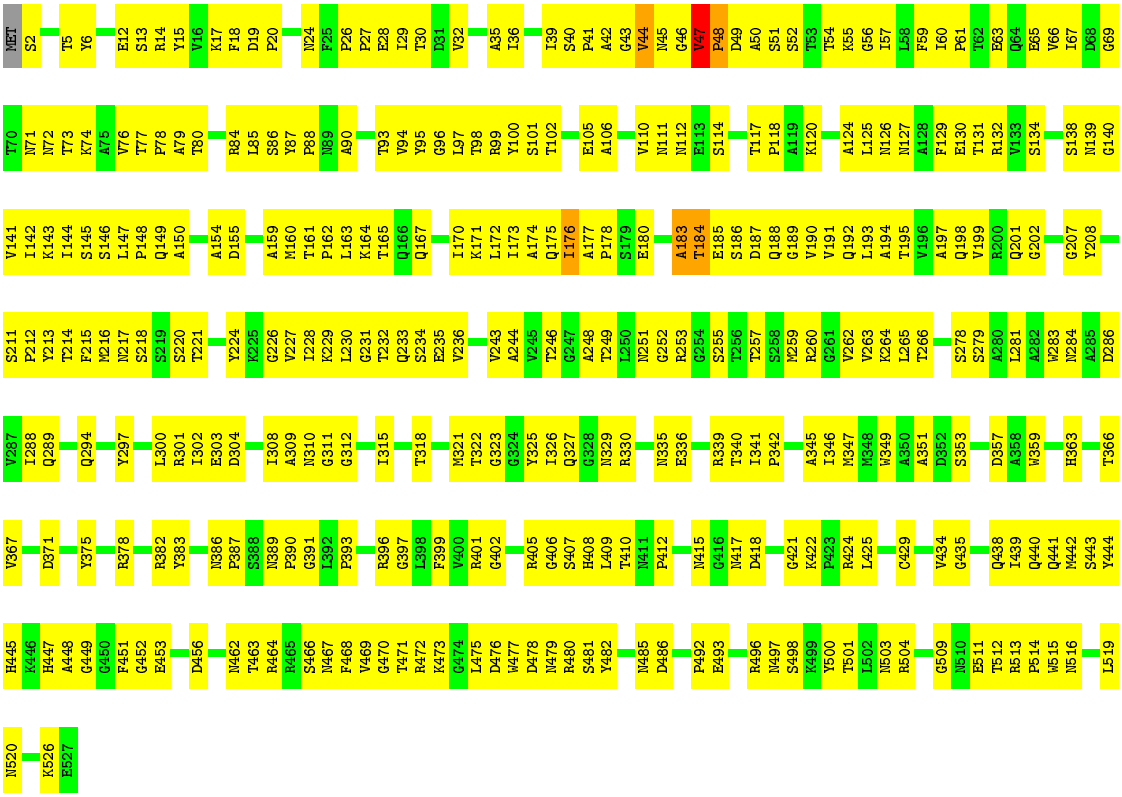


- Molecule 7: Short tail fiber protein gp12

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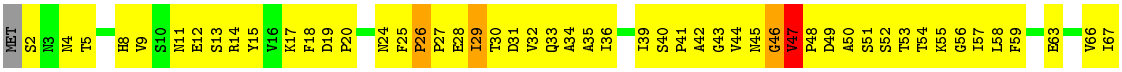

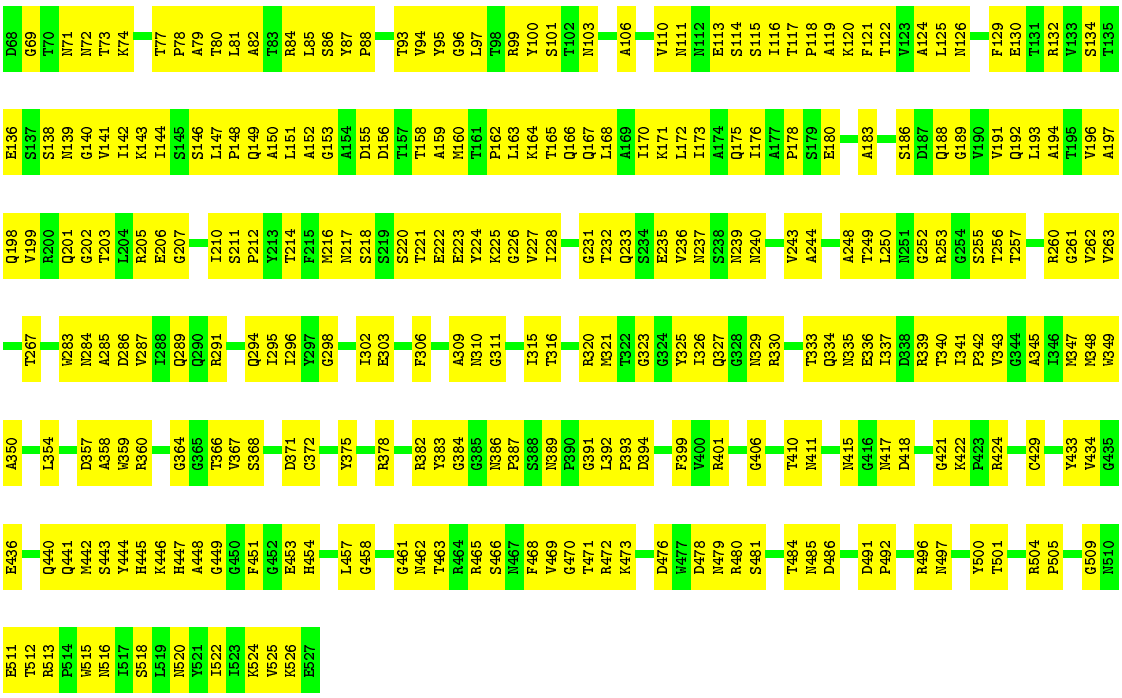

• Molecule 7: Short tail fiber protein gp12

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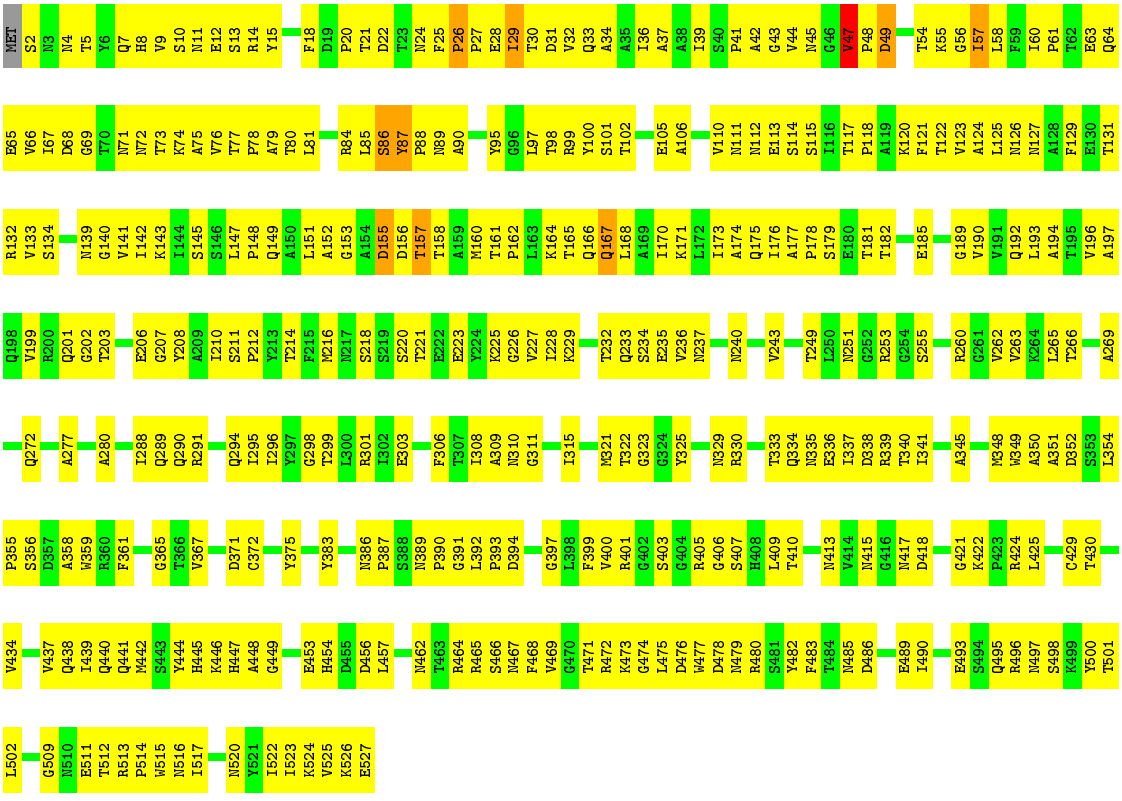

• Molecule 7: Short tail fiber protein gp12

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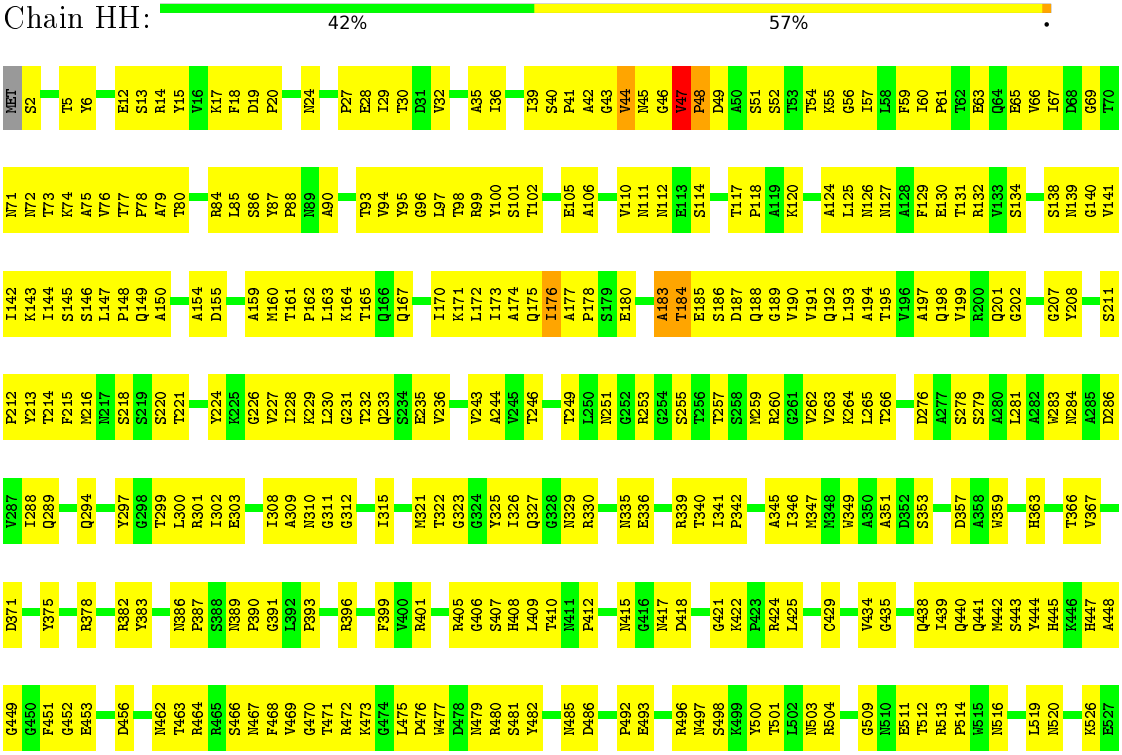


• Molecule 7: Short tail fiber protein gp12

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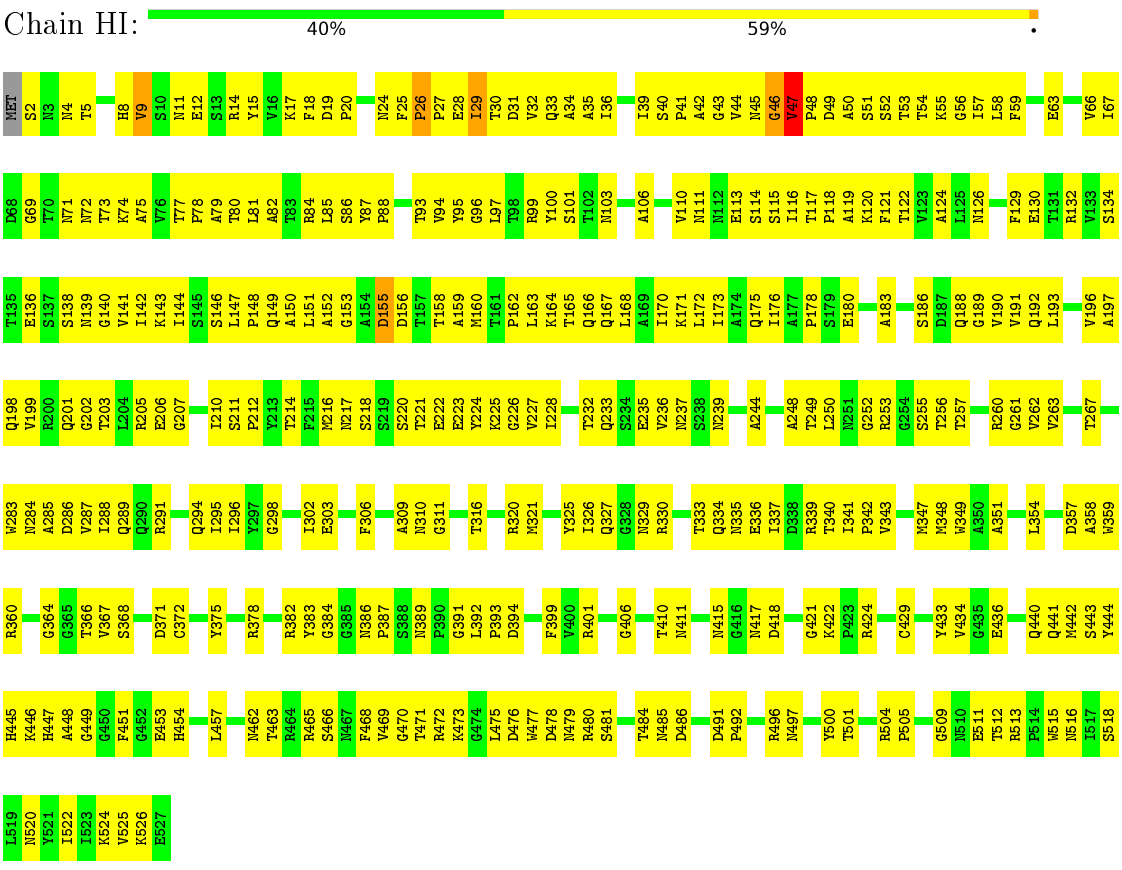

• Molecule 7: Short tail fiber protein gp12

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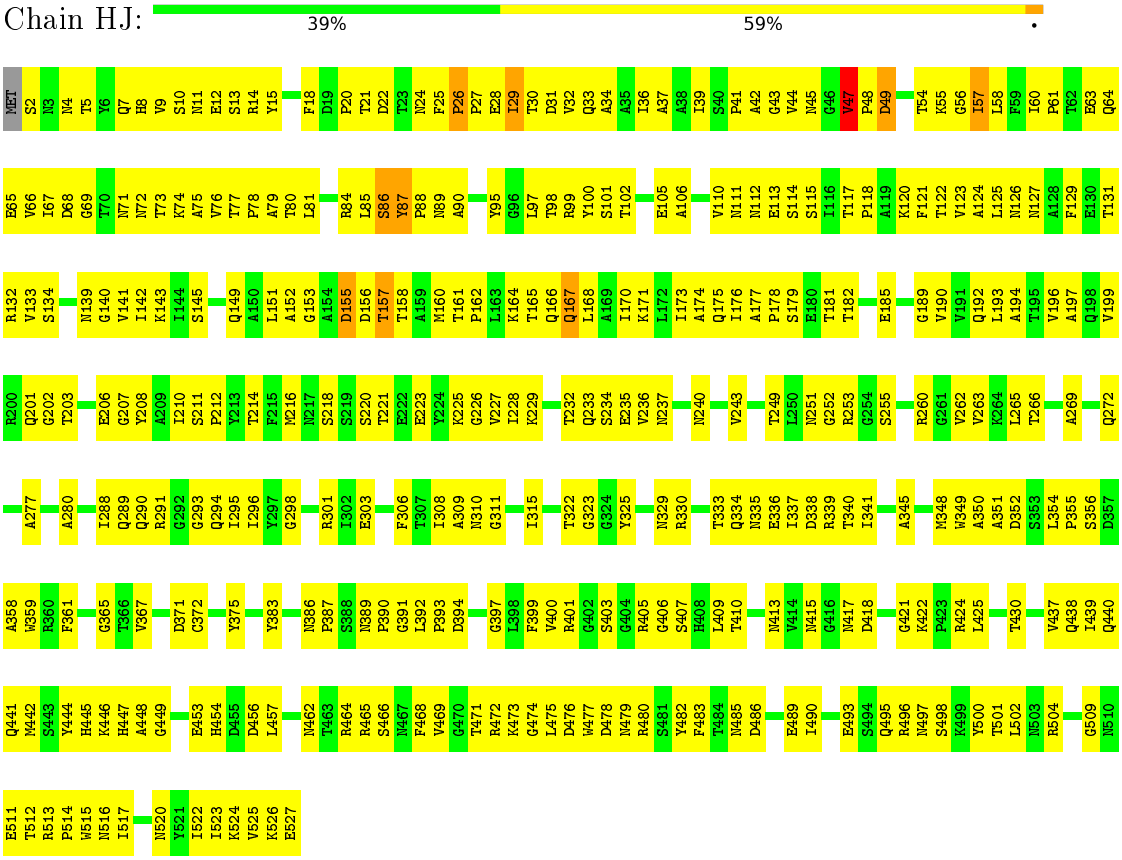


• Molecule 8: Tail tube protein gp19

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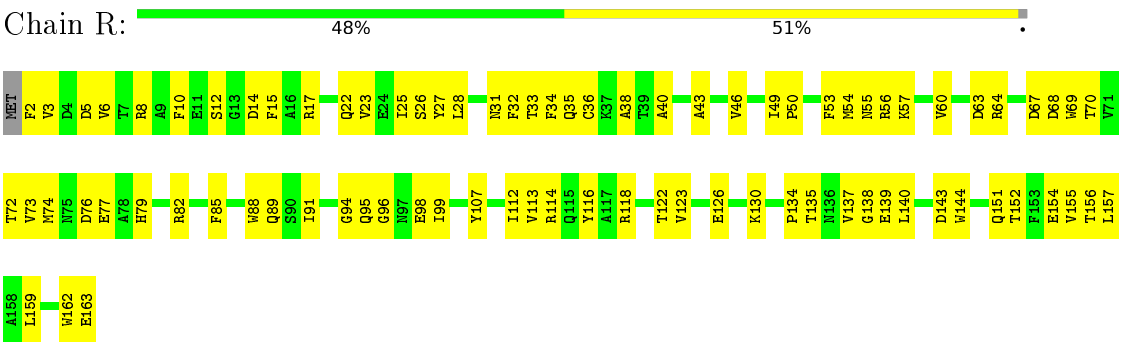


• Molecule 8: Tail tube protein gp19

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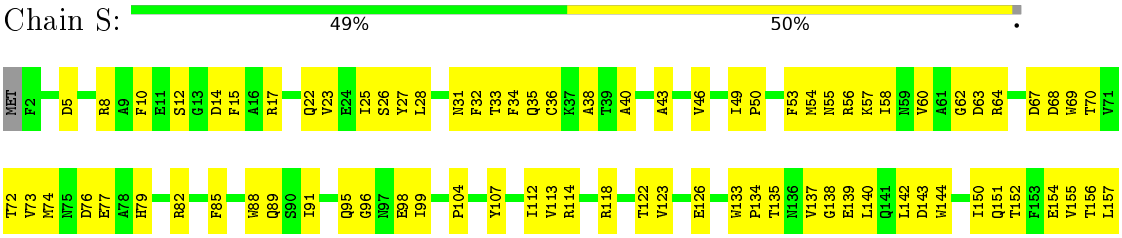

• Molecule 8: Tail tube protein gp19

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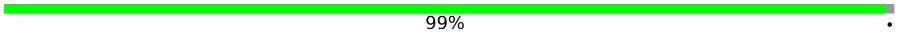

• Molecule 8: Tail tube protein gp19

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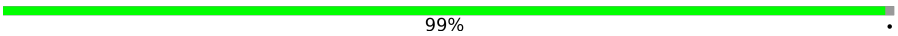

• Molecule 8: Tail tube protein gp19

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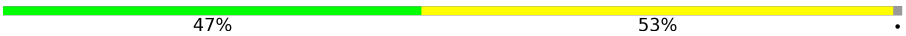


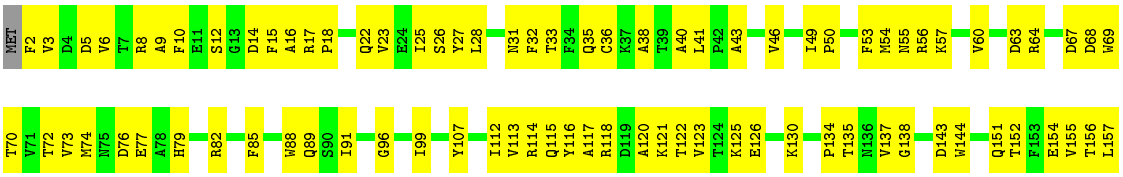

• Molecule 8: Tail tube protein gp19

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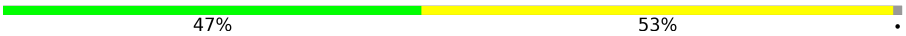


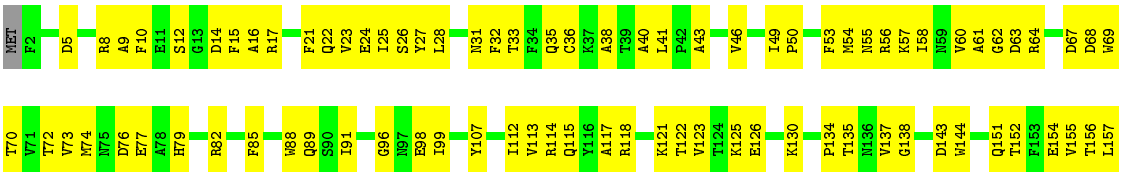

• Molecule 8: Tail tube protein gp19

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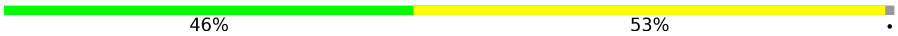


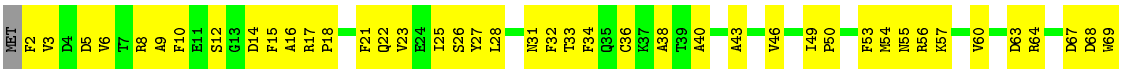

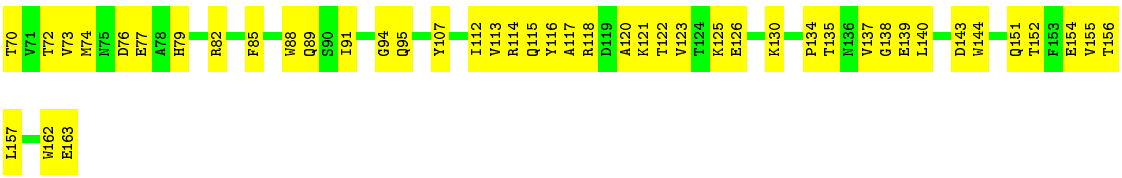


• Molecule 8: Tail tube protein gp19

Chain DF:

• Molecule 8: Tail tube protein gp19

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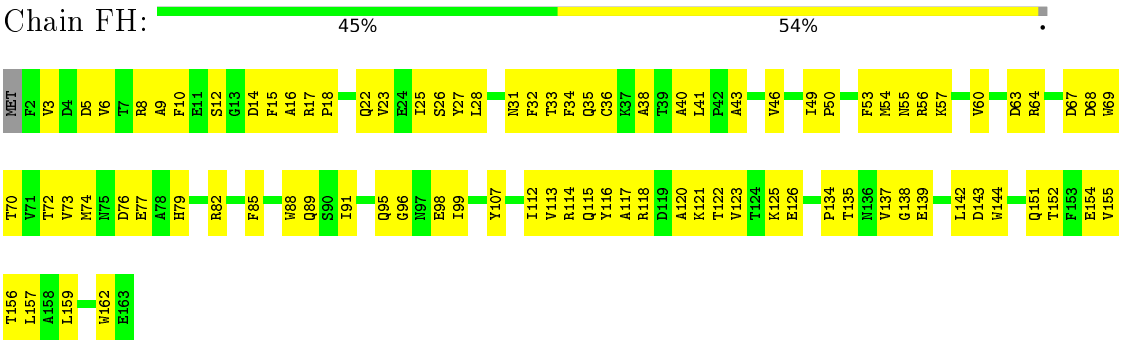


• Molecule 8: Tail tube protein gp19

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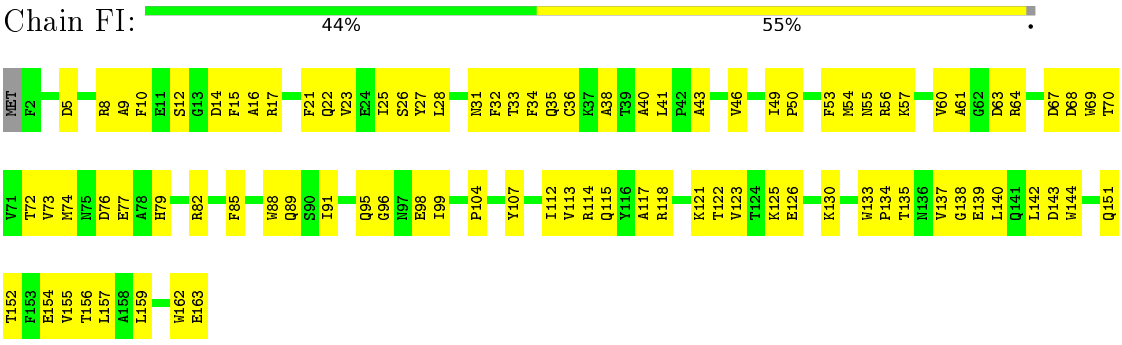


• Molecule 8: Tail tube protein gp19

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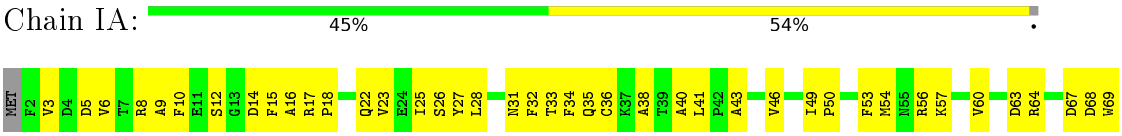

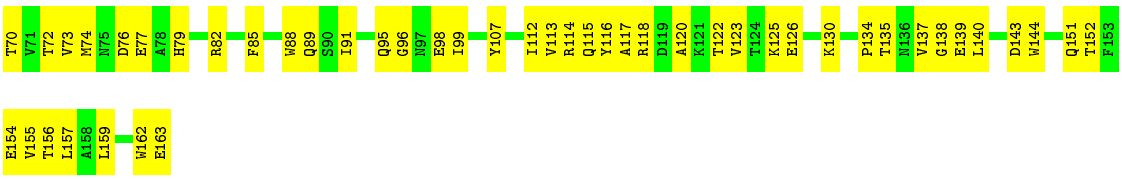


• Molecule 8: Tail tube protein gp19

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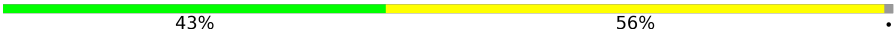


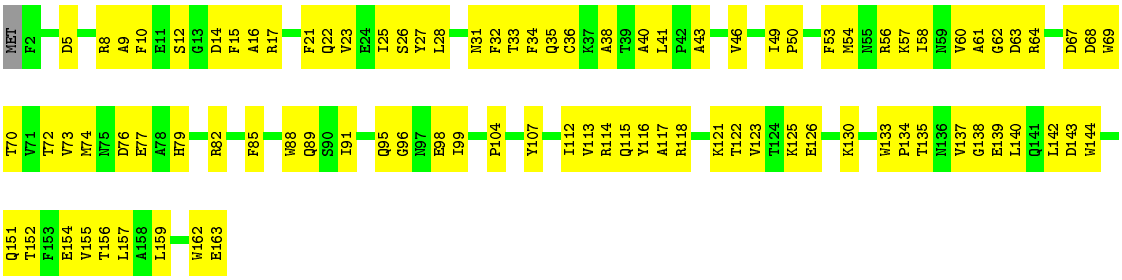


• Molecule 9: Baseplate wedge protein gp25

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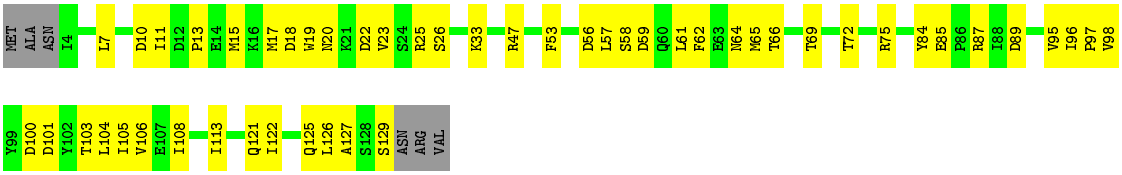


• Molecule 9: Baseplate wedge protein gp25

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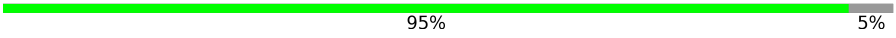


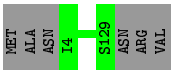


• Molecule 9: Baseplate wedge protein gp25

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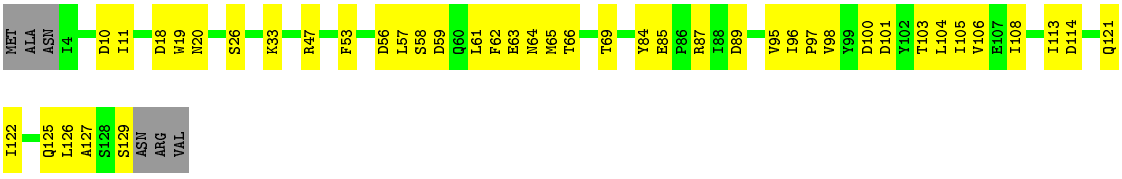


• Molecule 9: Baseplate wedge protein gp25

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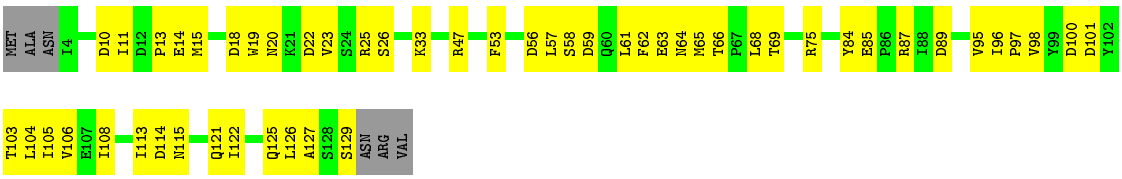


• Molecule 9: Baseplate wedge protein gp25

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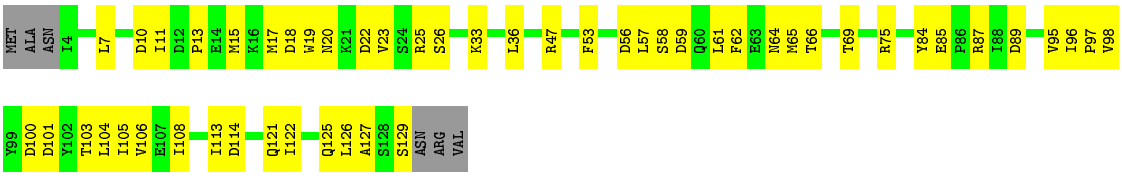


• Molecule 9: Baseplate wedge protein gp25

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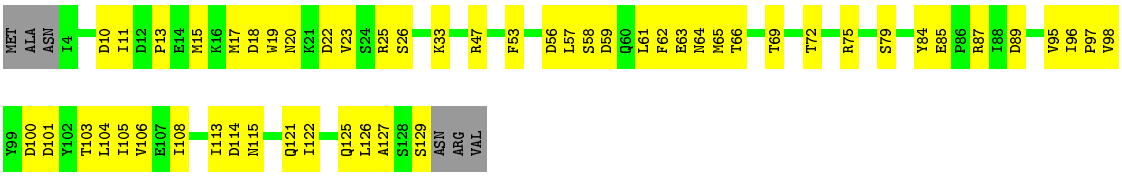


• Molecule 10: Baseplate tail-tube protein gp48

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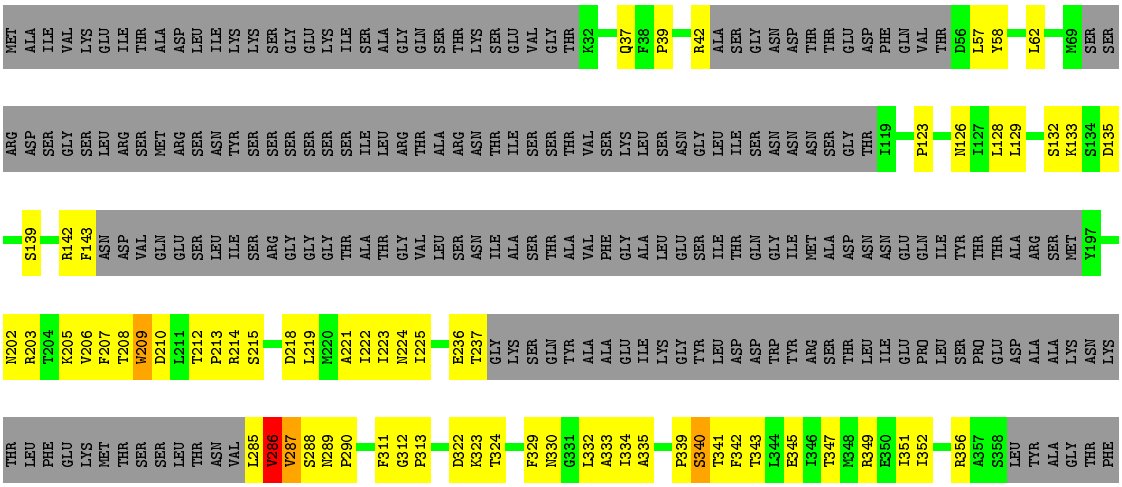
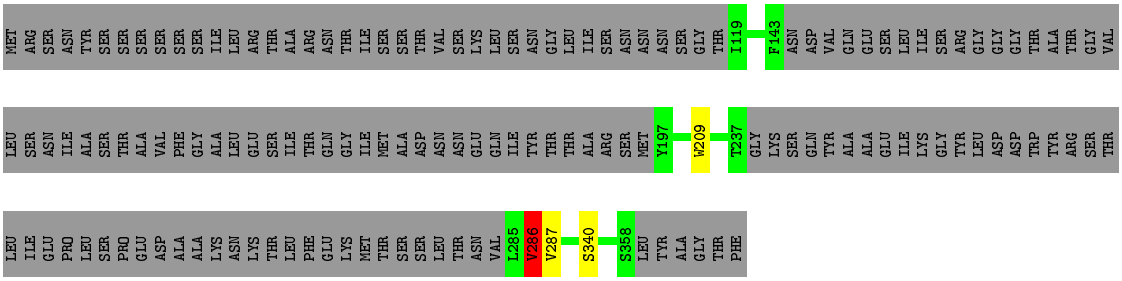



• Molecule 10: Baseplate tail-tube protein gp48

Chain r:



• Molecule 10: Baseplate tail-tube protein gp48

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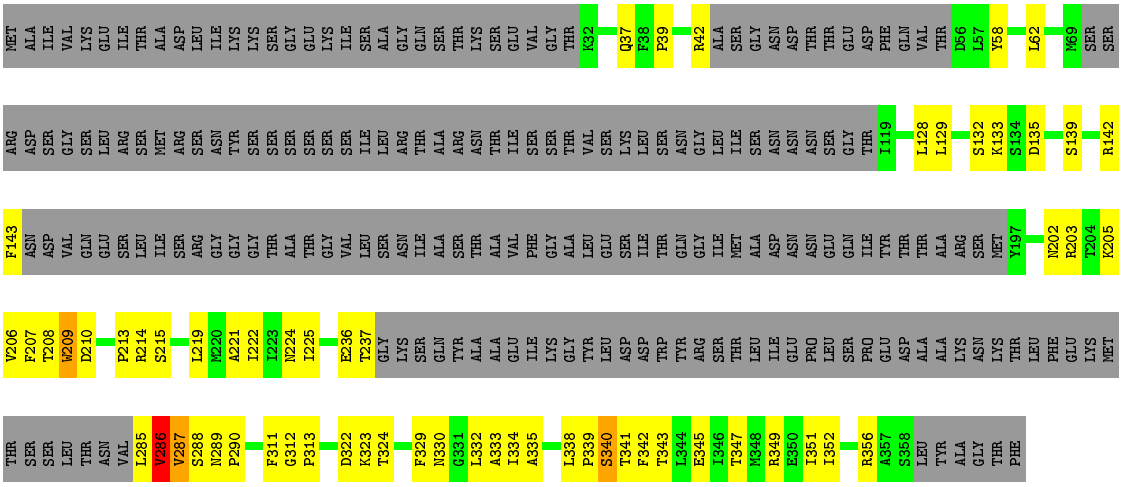

• Molecule 10: Baseplate tail-tube protein gp48

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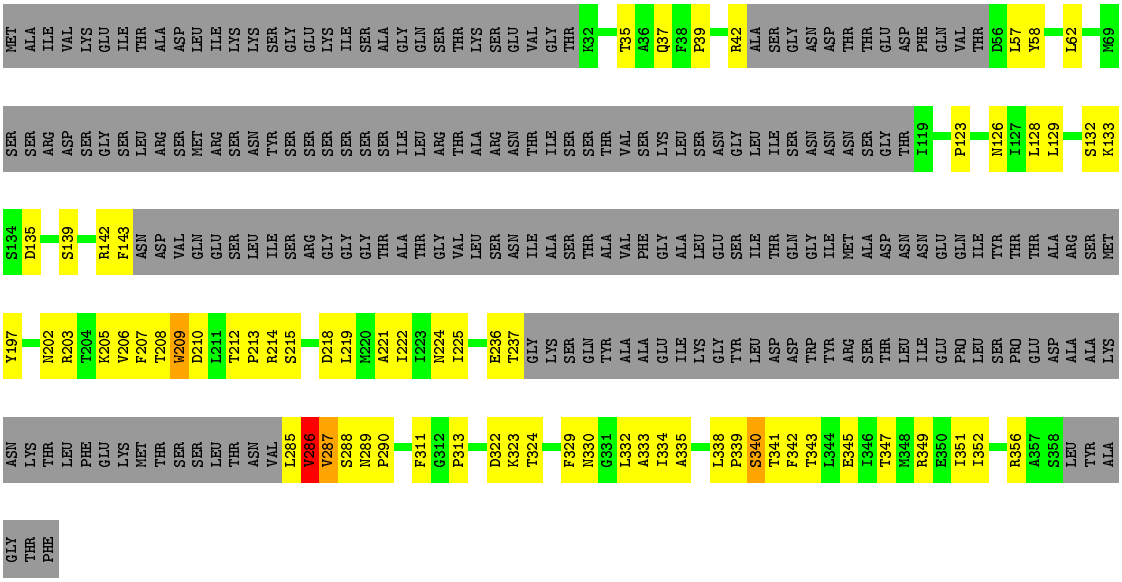

• Molecule 10: Baseplate tail-tube protein gp48

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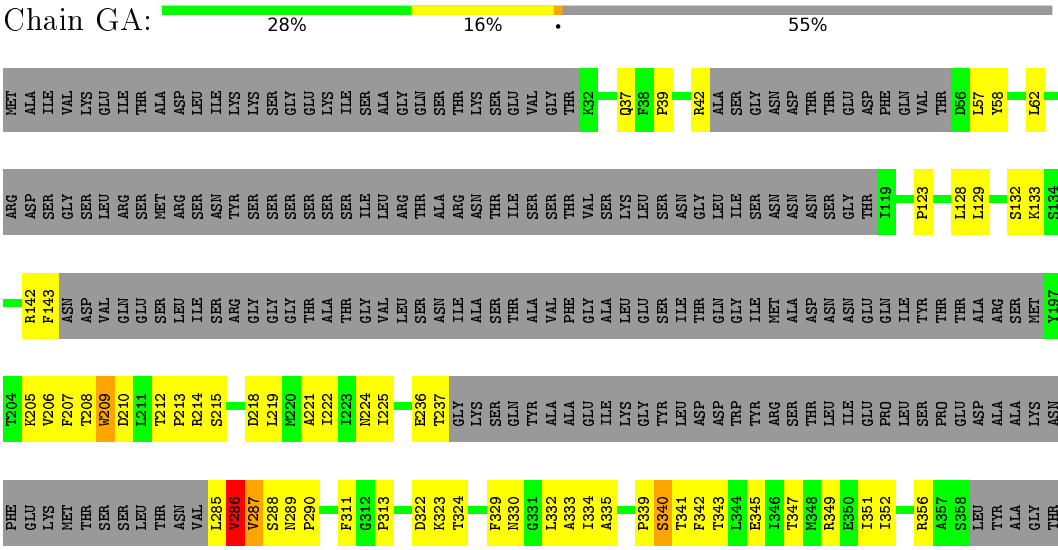


- Molecule 10: Baseplate tail-tube protein gp48

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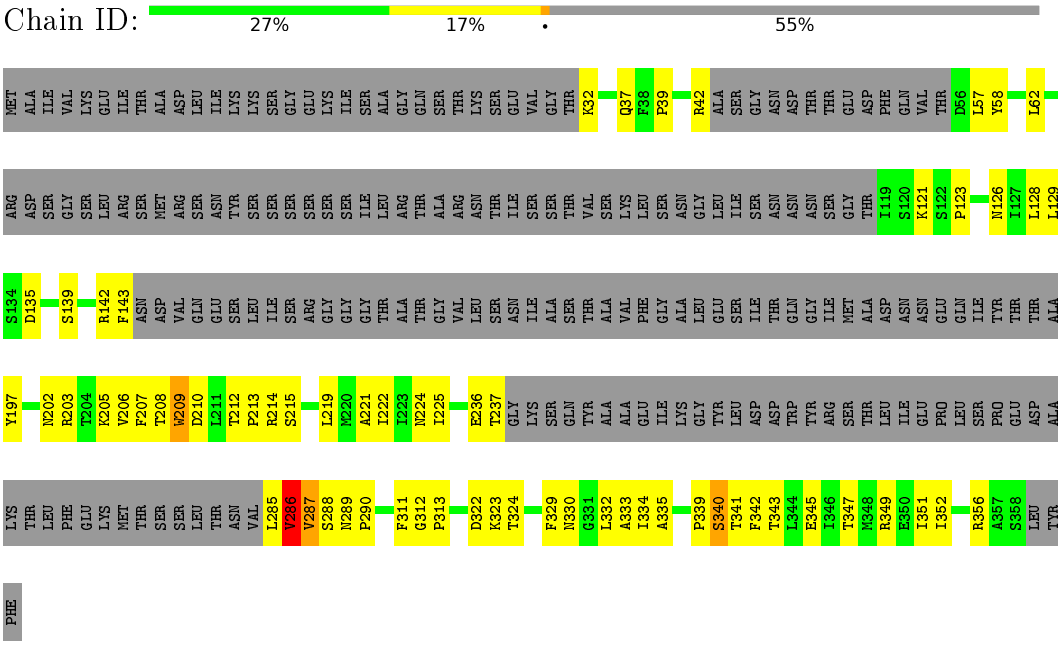
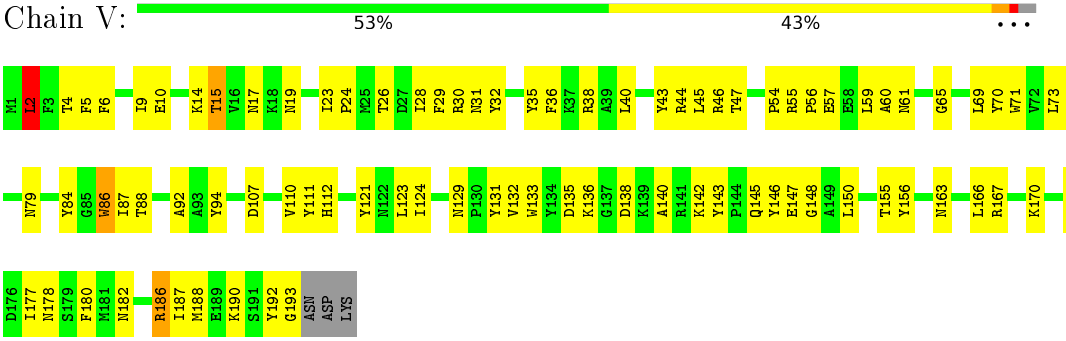


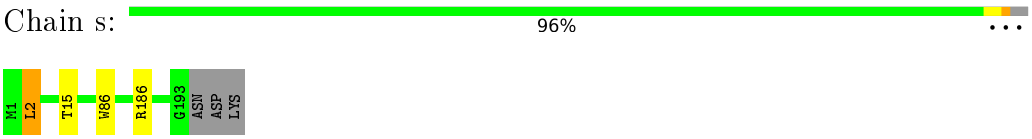

- Molecule 11: Baseplate wedge protein gp53

Chain V:



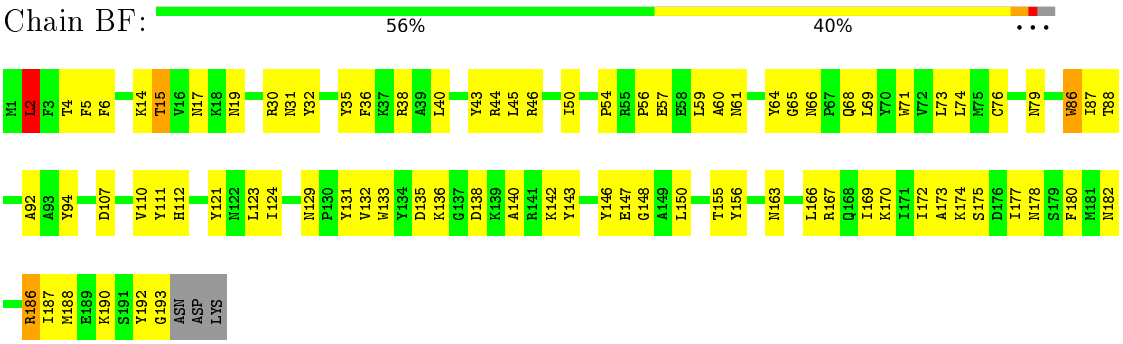
- Molecule 11: Baseplate wedge protein gp53

Chain s:



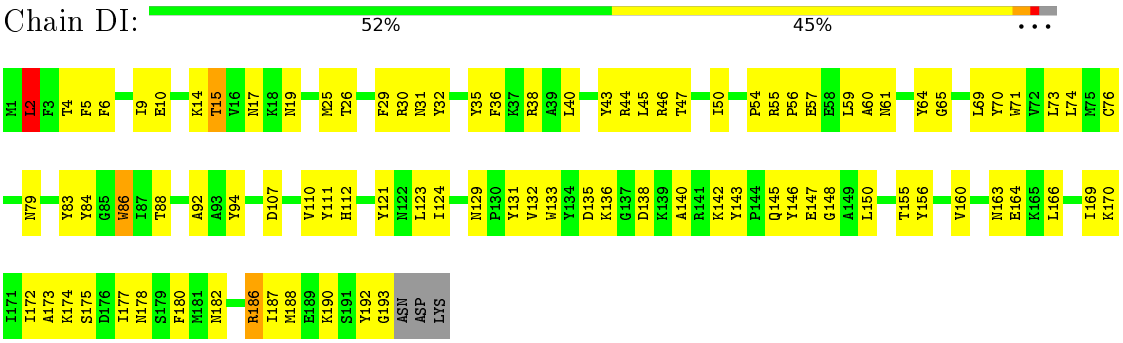

- Molecule 11: Baseplate wedge protein gp53

Chain BF:



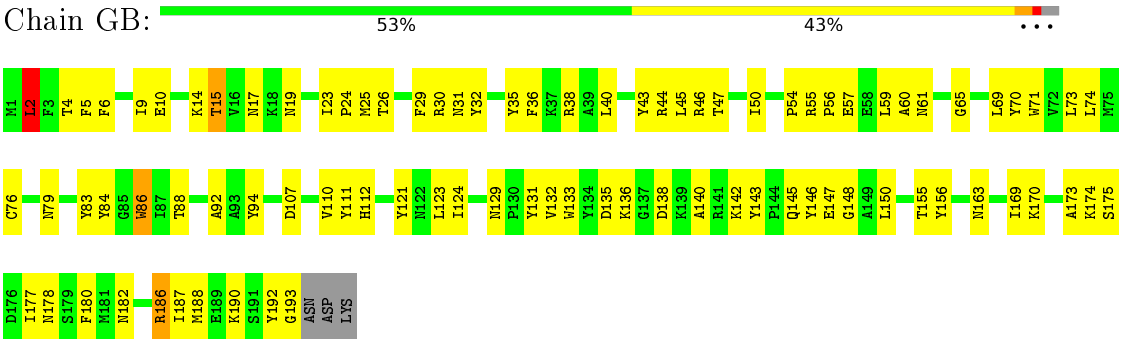

- Molecule 11: Baseplate wedge protein gp53

Chain DI:



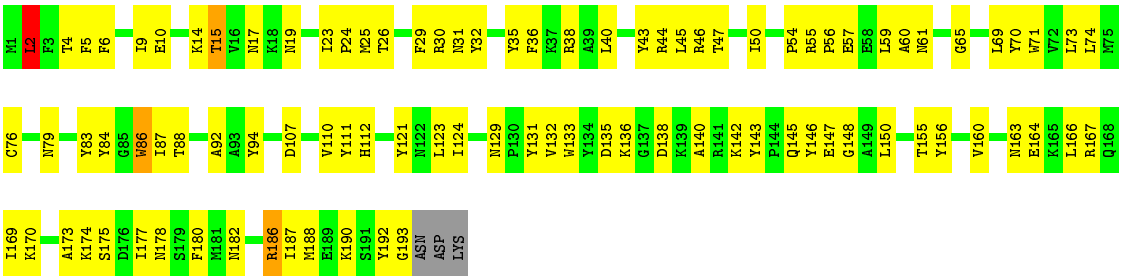

- Molecule 11: Baseplate wedge protein gp53

Chain GB:



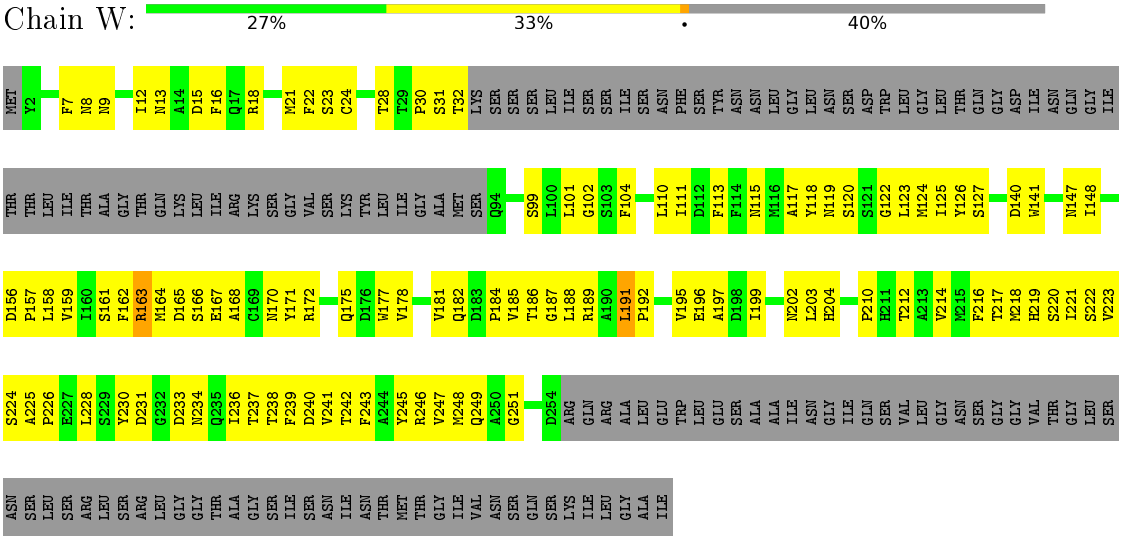

- Molecule 11: Baseplate wedge protein gp53

Chain IE:



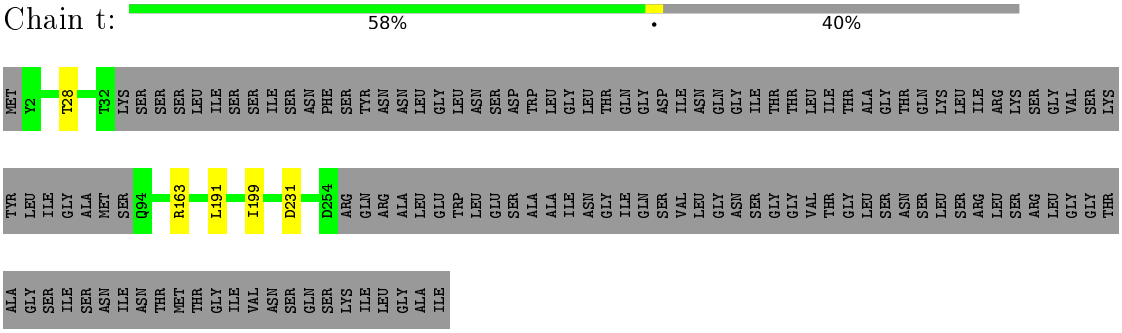
• Molecule 12: Baseplate tail-tube protein gp54

Chain W:



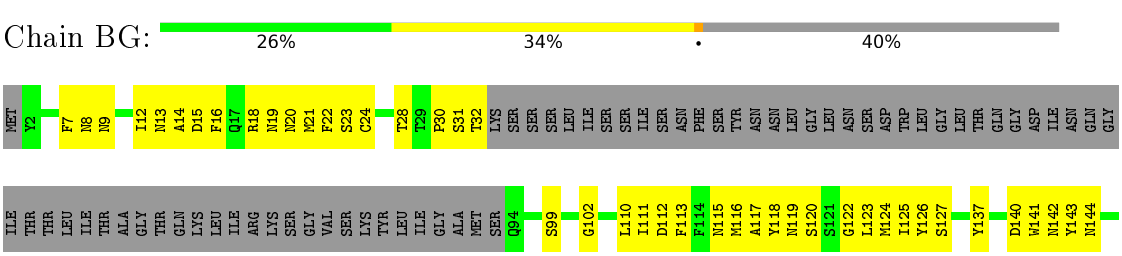

• Molecule 12: Baseplate tail-tube protein gp54

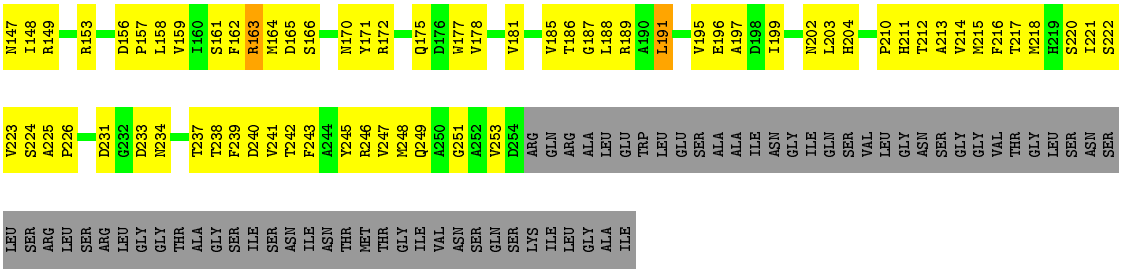
Chain t:




• Molecule 12: Baseplate tail-tube protein gp54

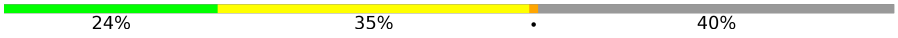
Chain BG:

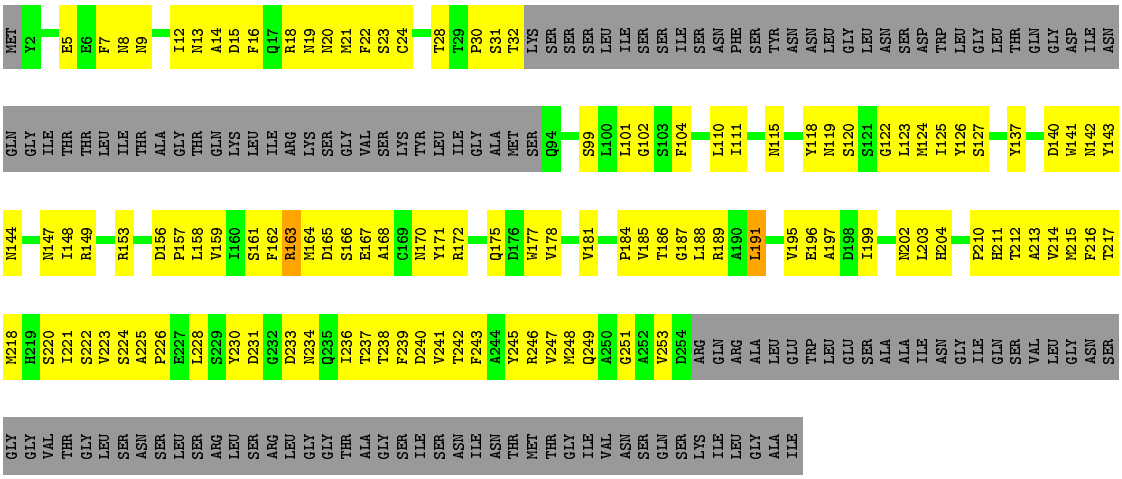





- Molecule 12: Baseplate tail-tube protein gp54

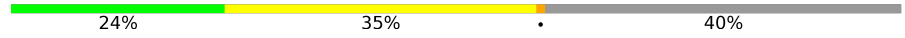
Chain DJ:

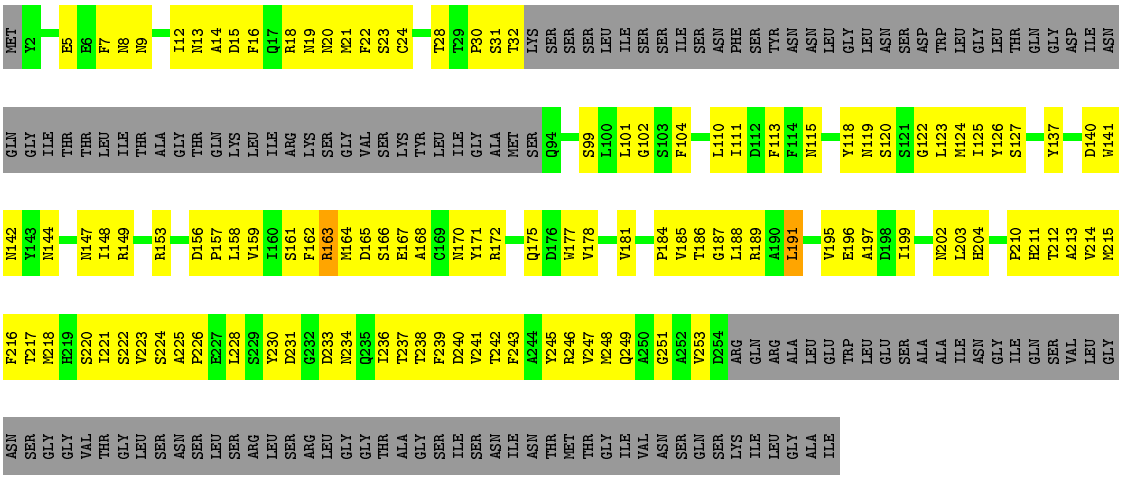



- Molecule 12: Baseplate tail-tube protein gp54

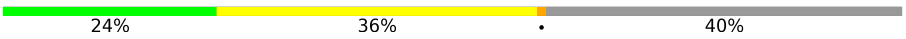
Chain GC:

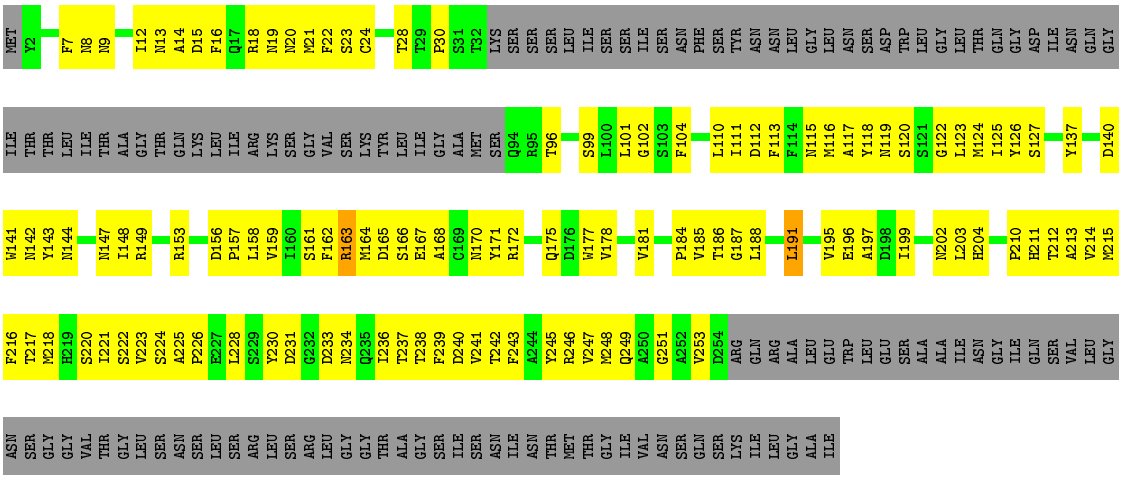



- Molecule 12: Baseplate tail-tube protein gp54

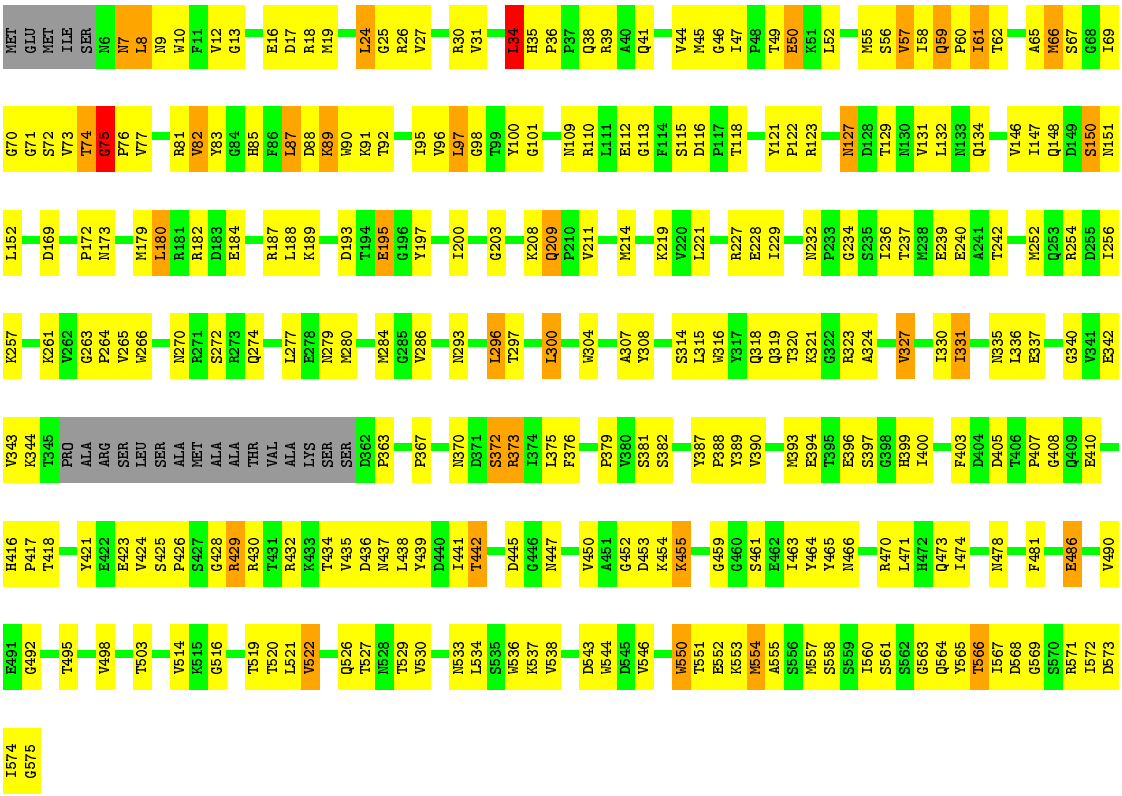
Chain IF:





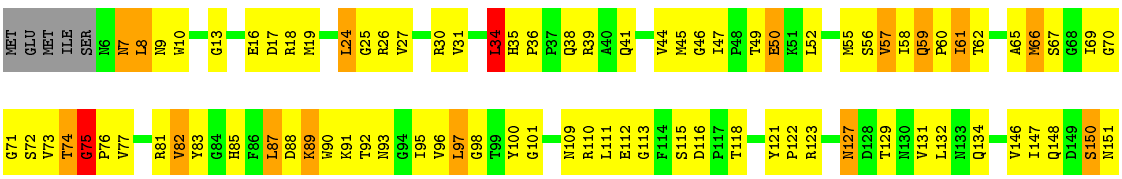
• Molecule 13: Peptidoglycan hydrolase gp5

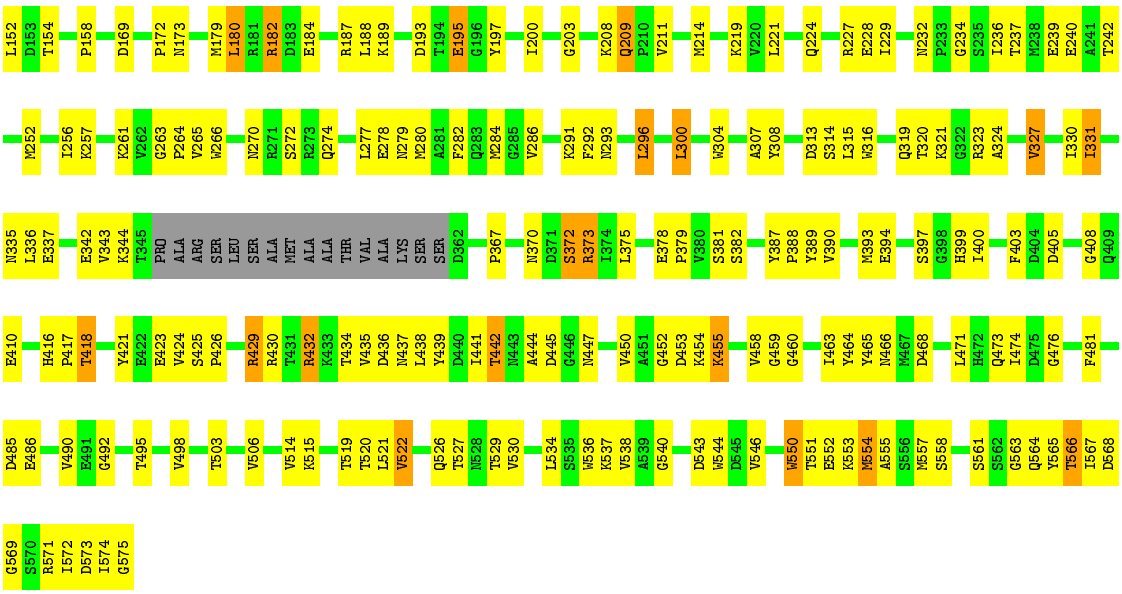
Chain YA:



• Molecule 13: Peptidoglycan hydrolase gp5

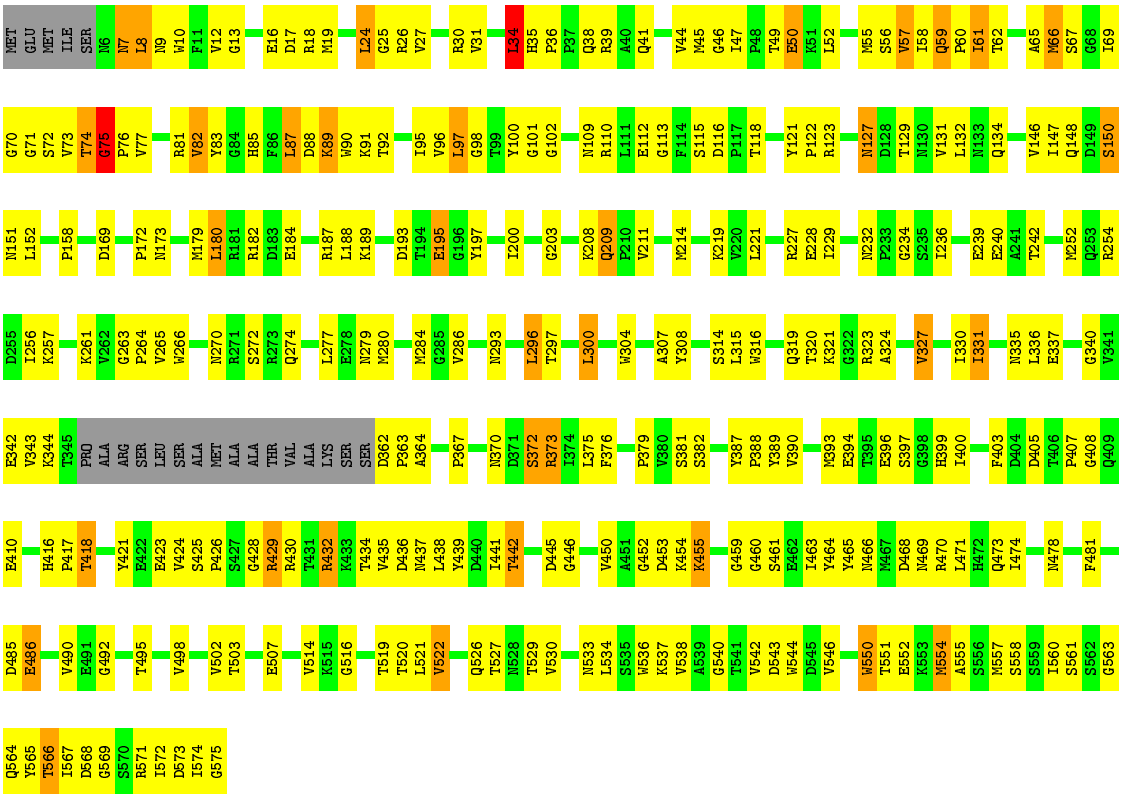
Chain YB:





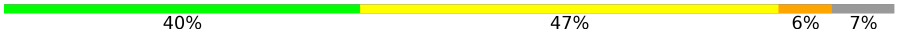
• Molecule 13: Peptidoglycan hydrolase gp5

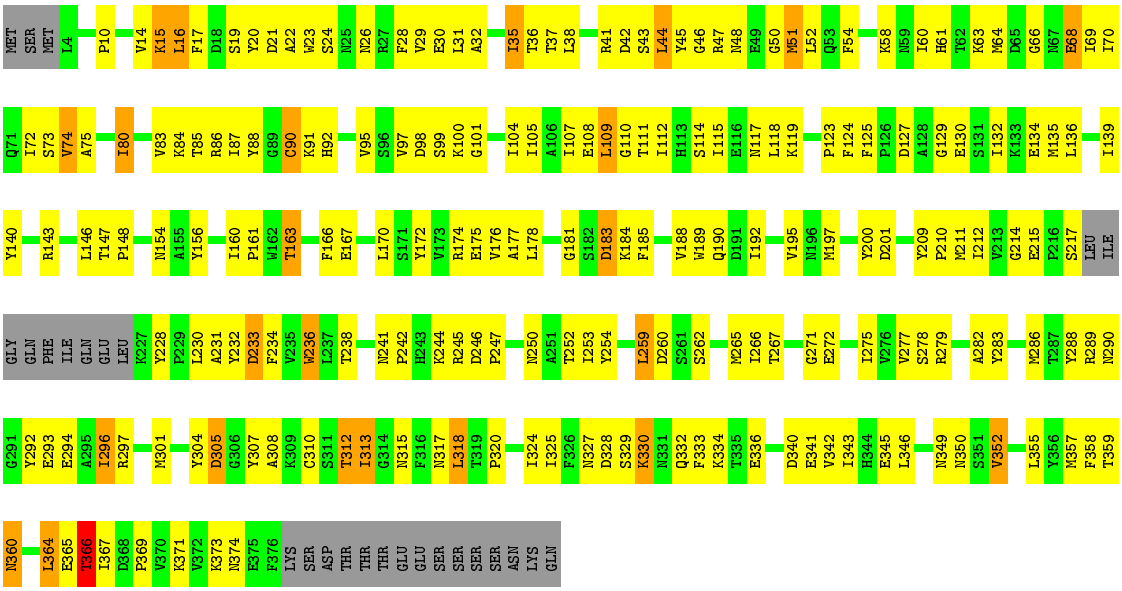
Chain YC:



• Molecule 14: Baseplate hub protein gp27

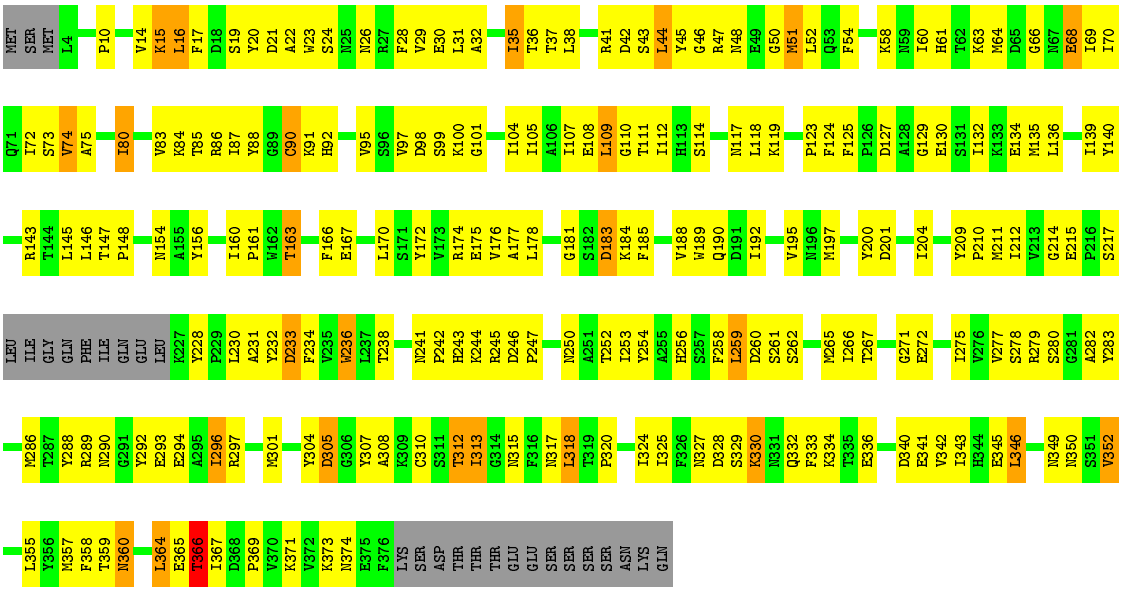
Chain YD:





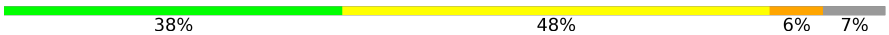
• Molecule 14: Baseplate hub protein gp27

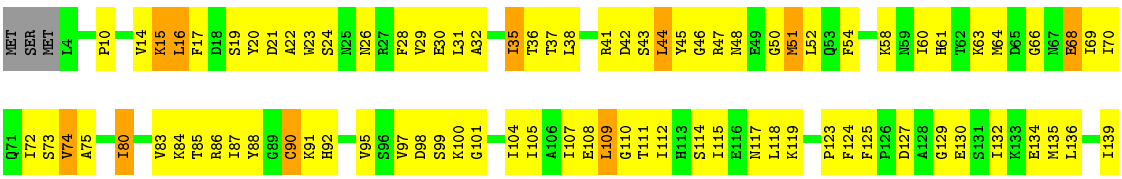
Chain YE:



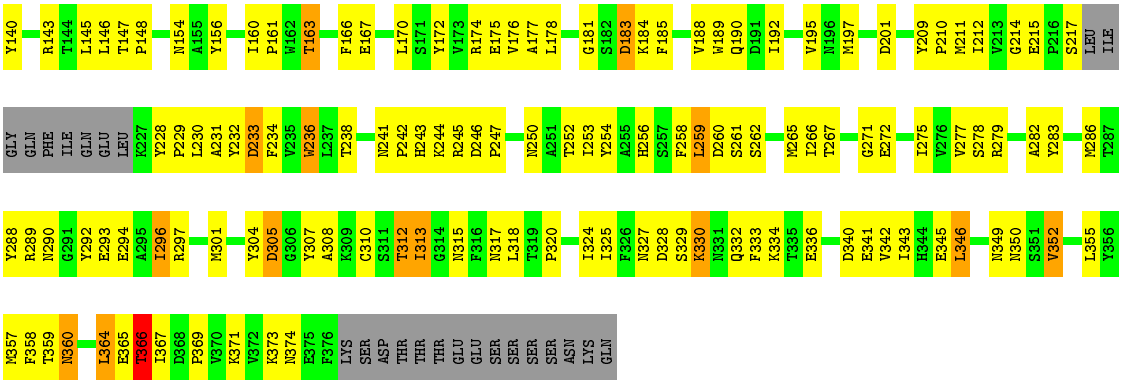
• Molecule 14: Baseplate hub protein gp27

Chain YF:



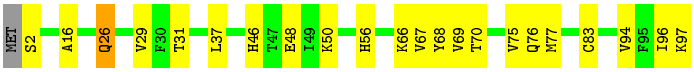



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM




- Molecule 15: Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region

Chain ZA:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | Not provided | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images used | 37913 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | Not provided | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | A | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | B | 0.71 | 1/5257 (0.0%) | 0.66 | 1/7144 (0.0%) |
| 1 | BH | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | BI | 0.71 | 1/5257 (0.0%) | 0.65 | 1/7144 (0.0%) |
| 1 | EA | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | EB | 0.71 | 1/5257 (0.0%) | 0.65 | 1/7144 (0.0%) |
| 1 | GD | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | GE | 0.71 | 1/5257 (0.0%) | 0.65 | 1/7144 (0.0%) |
| 1 | X | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | Y | 0.71 | 1/5257 (0.0%) | 0.66 | 1/7144 (0.0%) |
| 1 | u | 0.75 | 0/5337 | 0.66 | 1/7256 (0.0%) |
| 1 | v | 0.71 | 1/5257 (0.0%) | 0.65 | 1/7144 (0.0%) |
| 10 | BE | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 10 | DH | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 10 | GA | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 10 | ID | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 10 | U | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 10 | r | 0.77 | 1/1346 (0.1%) | 0.72 | 2/1821 (0.1%) |
| 11 | BF | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 11 | DI | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 11 | GB | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 11 | IE | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 11 | V | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 11 | s | 0.77 | 1/1643 (0.1%) | 0.76 | 3/2228 (0.1%) |
| 12 | BG | 0.62 | 1/1557 (0.1%) | 0.68 | 3/2118 (0.1%) |
| 12 | DJ | 0.62 | 1/1557 (0.1%) | 0.68 | 4/2118 (0.2%) |
| 12 | GC | 0.62 | 1/1557 (0.1%) | 0.68 | 3/2118 (0.1%) |
| 12 | IF | 0.63 | 1/1557 (0.1%) | 0.68 | 3/2118 (0.1%) |
| 12 | W | 0.62 | 1/1557 (0.1%) | 0.68 | 3/2118 (0.1%) |
| 12 | t | 0.62 | 1/1557 (0.1%) | 0.68 | 3/2118 (0.1%) |
| 13 | YA | 0.49 | 0/26166 | 0.60 | 24/35454 (0.1%) |
| 13 | YB | 0.49 | 0/26166 | 0.60 | 24/35454 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >2 | RMSZ | #\|Z\| >2 |
| 13 | YC | 0.49 | 0/26166 | 0.60 | 24/35454 (0.1%) |
| 14 | YD | 0.61 | 0/17880 | 0.64 | 6/24252 (0.0%) |
| 14 | YE | 0.61 | 0/17880 | 0.64 | 6/24252 (0.0%) |
| 14 | YF | 0.61 | 0/17880 | 0.64 | 6/24252 (0.0%) |
| 15 | ZA | 0.33 | 0/4344 | 0.54 | 0/5904 |
| 2 | BJ | 0.65 | 2/8405 (0.0%) | 0.73 | 2/11412 (0.0%) |
| 2 | C | 0.65 | 2/8405 (0.0%) | 0.74 | 2/11412 (0.0%) |
| 2 | EC | 0.65 | 2/8405 (0.0%) | 0.74 | 2/11412 (0.0%) |
| 2 | GF | 0.65 | 2/8405 (0.0%) | 0.74 | 2/11412 (0.0%) |
| 2 | Z | 0.65 | 2/8405 (0.0%) | 0.74 | 2/11412 (0.0%) |
| 2 | w | 0.65 | 2/8405 (0.0%) | 0.74 | 2/11412 (0.0%) |
| 3 | CA | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | CB | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 3 | D | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | E | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 3 | ED | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | EE | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 3 | GG | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | GH | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 3 | a | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | b | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 3 | x | 0.70 | 1/2709 (0.0%) | 0.57 | 0/3694 |
| 3 | y | 0.68 | 1/2736 (0.0%) | 0.62 | 0/3731 |
| 4 | AA | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | AB | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | CC | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | CD | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | CE | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | EF | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | EG | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | EH | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | F | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | G | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | GI | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | GJ | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | H | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | HA | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | c | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | d | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | e | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 4 | z | 0.28 | 0/2205 | 0.48 | 0/2988 |
| 5 | AC | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | AD | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >2 | RMSZ | #\|Z\| >2 |
| 5 | AE | 0.50 | 0/4778 | 0.70 | 3/6513 (0.0%) |
| 5 | CF | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | CG | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |
| 5 | CH | 0.50 | 0/4778 | 0.70 | 3/6513 (0.0%) |
| 5 | EI | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | EJ | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |
| 5 | FA | 0.50 | 0/4778 | 0.70 | 3/6513 (0.0%) |
| 5 | HB | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | HC | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |
| 5 | HD | 0.50 | 0/4778 | 0.70 | 4/6513 (0.1%) |
| 5 | I | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | J | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |
| 5 | K | 0.50 | 0/4778 | 0.70 | 4/6513 (0.1%) |
| 5 | f | 0.48 | 0/4778 | 0.68 | 2/6513 (0.0%) |
| 5 | g | 0.49 | 1/4778 (0.0%) | 0.69 | 5/6513 (0.1%) |
| 5 | h | 0.50 | 0/4778 | 0.70 | 4/6513 (0.1%) |
| 6 | AF | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | AG | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | AH | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | CI | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | CJ | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | DA | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | FB | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | FC | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | FD | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | HE | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | HF | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | HG | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | L | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | M | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | N | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | i | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | j | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 6 | k | 0.34 | 0/1700 | 0.51 | 0/2318 |
| 7 | AI | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | AJ | 0.39 | 1/4016 (0.0%) | 0.61 | 0/5464 |
| 7 | BA | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | DB | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | DC | 0.39 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | DD | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | FE | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | FF | 0.39 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | FG | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >2 | RMSZ | #\|Z\| >2 |
| 7 | HH | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | HI | 0.39 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | HJ | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | O | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | P | 0.39 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | Q | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 7 | l | 0.39 | 0/4016 | 0.61 | 0/5464 |
| 7 | m | 0.39 | 1/4016 (0.0%) | 0.61 | 0/5464 |
| 7 | n | 0.40 | 1/4016 (0.0%) | 0.60 | 0/5464 |
| 8 | BB | 0.45 | 0/1325 | 0.58 | 0/1797 |
| 8 | BC | 0.45 | 0/1325 | 0.58 | 0/1797 |
| 8 | DE | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | DF | 0.45 | 0/1325 | 0.58 | 0/1797 |
| 8 | FH | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | FI | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | IA | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | IB | 0.45 | 0/1325 | 0.58 | 0/1797 |
| 8 | R | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | S | 0.45 | 0/1325 | 0.58 | 0/1797 |
| 8 | o | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 8 | p | 0.44 | 0/1325 | 0.58 | 0/1797 |
| 9 | BD | 0.55 | 0/1027 | 0.59 | 0/1392 |
| 9 | DG | 0.55 | 0/1027 | 0.59 | 0/1392 |
| 9 | FJ | 0.55 | 0/1027 | 0.59 | 0/1392 |
| 9 | IC | 0.55 | 0/1027 | 0.59 | 0/1392 |
| 9 | T | 0.55 | 0/1027 | 0.59 | 0/1392 |
| 9 | q | 0.55 | 0/1027 | 0.59 | 0/1392 |
| All | All | 0.55 | 66/561066 (0.0%) | 0.63 | 226/762456 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 8 |
| 1 | BH | 0 | 1 |
| 1 | BI | 0 | 8 |
| 1 | EA | 0 | 1 |
| 1 | EB | 0 | 8 |
| 1 | GD | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | GE | 0 | 8 |
| 1 | X | 0 | 1 |
| 1 | Y | 0 | 8 |
| 1 | u | 0 | 1 |
| 1 | v | 0 | 8 |
| 10 | BE | 0 | 1 |
| 10 | DH | 0 | 1 |
| 10 | GA | 0 | 1 |
| 10 | ID | 0 | 1 |
| 10 | U | 0 | 1 |
| 10 | r | 0 | 1 |
| 11 | BF | 0 | 1 |
| 11 | DI | 0 | 1 |
| 11 | GB | 0 | 1 |
| 11 | IE | 0 | 1 |
| 11 | V | 0 | 1 |
| 11 | s | 0 | 1 |
| 13 | YA | 0 | 7 |
| 13 | YB | 0 | 7 |
| 13 | YC | 0 | 7 |
| 14 | YD | 0 | 6 |
| 14 | YE | 0 | 6 |
| 14 | YF | 0 | 6 |
| 2 | BJ | 0 | 38 |
| 2 | C | 0 | 38 |
| 2 | EC | 0 | 38 |
| 2 | GF | 0 | 38 |
| 2 | Z | 0 | 38 |
| 2 | w | 0 | 38 |
| 3 | CA | 0 | 2 |
| 3 | CB | 0 | 3 |
| 3 | D | 0 | 2 |
| 3 | E | 0 | 3 |
| 3 | ED | 0 | 2 |
| 3 | EE | 0 | 3 |
| 3 | GG | 0 | 2 |
| 3 | GH | 0 | 3 |
| 3 | a | 0 | 2 |
| 3 | b | 0 | 3 |
| 3 | x | 0 | 2 |
| 3 | y | 0 | 3 |
| 5 | AC | 0 | 17 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 5 | AD | 0 | 13 |
| 5 | AE | 0 | 16 |
| 5 | CF | 0 | 17 |
| 5 | CG | 0 | 13 |
| 5 | CH | 0 | 16 |
| 5 | EI | 0 | 17 |
| 5 | EJ | 0 | 13 |
| 5 | FA | 0 | 16 |
| 5 | HB | 0 | 17 |
| 5 | HC | 0 | 13 |
| 5 | HD | 0 | 16 |
| 5 | I | 0 | 17 |
| 5 | J | 0 | 13 |
| 5 | K | 0 | 16 |
| 5 | f | 0 | 17 |
| 5 | g | 0 | 13 |
| 5 | h | 0 | 16 |
| 6 | AF | 0 | 3 |
| 6 | AG | 0 | 3 |
| 6 | AH | 0 | 3 |
| 6 | CI | 0 | 3 |
| 6 | CJ | 0 | 3 |
| 6 | DA | 0 | 3 |
| 6 | FB | 0 | 3 |
| 6 | FC | 0 | 3 |
| 6 | FD | 0 | 3 |
| 6 | HE | 0 | 3 |
| 6 | HF | 0 | 3 |
| 6 | HG | 0 | 3 |
| 6 | L | 0 | 3 |
| 6 | M | 0 | 3 |
| 6 | N | 0 | 3 |
| 6 | i | 0 | 3 |
| 6 | j | 0 | 3 |
| 6 | k | 0 | 3 |
| 7 | AI | 0 | 4 |
| 7 | AJ | 0 | 6 |
| 7 | BA | 0 | 5 |
| 7 | DB | 0 | 4 |
| 7 | DC | 0 | 6 |
| 7 | DD | 0 | 5 |
| 7 | FE | 0 | 4 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 7 | FF | 0 | 6 |
| 7 | FG | 0 | 5 |
| 7 | HH | 0 | 4 |
| 7 | HI | 0 | 6 |
| 7 | HJ | 0 | 5 |
| 7 | O | 0 | 4 |
| 7 | P | 0 | 6 |
| 7 | Q | 0 | 5 |
| 7 | l | 0 | 4 |
| 7 | m | 0 | 6 |
| 7 | n | 0 | 5 |
| All | All | 0 | 783 |

All (66) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | CA | 258 | PHE | C-N | -20.87 | 0.94 | 1.34 |
| 3 | ED | 258 | PHE | C-N | -20.85 | 0.94 | 1.34 |
| 3 | GG | 258 | PHE | C-N | -20.84 | 0.94 | 1.34 |
| 3 | x | 258 | PHE | C-N | -20.84 | 0.94 | 1.34 |
| 3 | a | 258 | PHE | C-N | -20.82 | 0.94 | 1.34 |
| 3 | D | 258 | PHE | C-N | -20.82 | 0.94 | 1.34 |
| 1 | v | 307 | ASP | C-N | -12.66 | 1.10 | 1.34 |
| 1 | GE | 307 | ASP | C-N | -12.65 | 1.10 | 1.34 |
| 1 | Y | 307 | ASP | C-N | -12.65 | 1.10 | 1.34 |
| 1 | B | 307 | ASP | C-N | -12.64 | 1.10 | 1.34 |
| 1 | EB | 307 | ASP | C-N | -12.60 | 1.10 | 1.34 |
| 1 | BI | 307 | ASP | C-N | -12.60 | 1.10 | 1.34 |
| 2 | w | 652 | MET | C-N | -10.23 | 1.10 | 1.34 |
| 2 | C | 652 | MET | C-N | -10.23 | 1.10 | 1.34 |
| 2 | EC | 652 | MET | C-N | -10.22 | 1.10 | 1.34 |
| 2 | Z | 652 | MET | C-N | -10.22 | 1.10 | 1.34 |
| 2 | GF | 652 | MET | C-N | -10.22 | 1.10 | 1.34 |
| 2 | BJ | 652 | MET | C-N | -10.21 | 1.10 | 1.34 |
| 7 | Q | 26 | PRO | C-N | -8.32 | 1.18 | 1.34 |
| 7 | FG | 26 | PRO | C-N | -8.30 | 1.18 | 1.34 |
| 7 | n | 26 | PRO | C-N | -8.29 | 1.18 | 1.34 |
| 7 | HJ | 26 | PRO | C-N | -8.28 | 1.18 | 1.34 |
| 7 | DD | 26 | PRO | C-N | -8.28 | 1.18 | 1.34 |
| 7 | BA | 26 | PRO | C-N | -8.25 | 1.18 | 1.34 |
| 11 | BF | 86 | TRP | CB-CG | -7.02 | 1.37 | 1.50 |
| 11 | V | 86 | TRP | CB-CG | -6.99 | 1.37 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | s | 86 | TRP | CB-CG | -6.97 | 1.37 | 1.50 |
| 11 | IE | 86 | TRP | CB-CG | -6.96 | 1.37 | 1.50 |
| 11 | GB | 86 | TRP | CB-CG | -6.96 | 1.37 | 1.50 |
| 11 | DI | 86 | TRP | CB-CG | -6.95 | 1.37 | 1.50 |
| 5 | g | 531 | ASN | C-N | -6.59 | 1.18 | 1.34 |
| 5 | J | 531 | ASN | C-N | -6.59 | 1.19 | 1.34 |
| 5 | AD | 531 | ASN | C-N | -6.58 | 1.19 | 1.34 |
| 5 | HC | 531 | ASN | C-N | -6.58 | 1.19 | 1.34 |
| 5 | CG | 531 | ASN | C-N | -6.56 | 1.19 | 1.34 |
| 5 | EJ | 531 | ASN | C-N | -6.53 | 1.19 | 1.34 |
| 7 | DC | 26 | PRO | C-N | -6.14 | 1.22 | 1.34 |
| 7 | AJ | 26 | PRO | C-N | -6.13 | 1.22 | 1.34 |
| 7 | HI | 26 | PRO | C-N | -6.13 | 1.22 | 1.34 |
| 7 | FF | 26 | PRO | C-N | -6.13 | 1.22 | 1.34 |
| 7 | P | 26 | PRO | C-N | -6.11 | 1.22 | 1.34 |
| 7 | m | 26 | PRO | C-N | -6.09 | 1.22 | 1.34 |
| 10 | BE | 209 | TRP | CB-CG | -5.86 | 1.39 | 1.50 |
| 10 | GA | 209 | TRP | CB-CG | -5.84 | 1.39 | 1.50 |
| 10 | U | 209 | TRP | CB-CG | -5.83 | 1.39 | 1.50 |
| 10 | r | 209 | TRP | CB-CG | -5.82 | 1.39 | 1.50 |
| 10 | DH | 209 | TRP | CB-CG | -5.80 | 1.39 | 1.50 |
| 10 | ID | 209 | TRP | CB-CG | -5.80 | 1.39 | 1.50 |
| 2 | GF | 714 | TYR | CD2-CE2 | -5.74 | 1.30 | 1.39 |
| 2 | BJ | 714 | TYR | CD2-CE2 | -5.74 | 1.30 | 1.39 |
| 2 | Z | 714 | TYR | CD2-CE2 | -5.72 | 1.30 | 1.39 |
| 2 | EC | 714 | TYR | CD2-CE2 | -5.72 | 1.30 | 1.39 |
| 2 | C | 714 | TYR | CD2-CE2 | -5.70 | 1.30 | 1.39 |
| 2 | w | 714 | TYR | CD2-CE2 | -5.64 | 1.30 | 1.39 |
| 12 | IF | 28 | THR | C-N | -5.60 | 1.21 | 1.34 |
| 12 | GC | 28 | THR | C-N | -5.56 | 1.21 | 1.34 |
| 12 | BG | 28 | THR | C-N | -5.55 | 1.21 | 1.34 |
| 12 | W | 28 | THR | C-N | -5.54 | 1.21 | 1.34 |
| 12 | DJ | 28 | THR | C-N | -5.54 | 1.21 | 1.34 |
| 12 | t | 28 | THR | C-N | -5.54 | 1.21 | 1.34 |
| 3 | b | 81 | VAL | C-N | -5.37 | 1.21 | 1.34 |
| 3 | GH | 81 | VAL | C-N | -5.36 | 1.21 | 1.34 |
| 3 | CB | 81 | VAL | C-N | -5.35 | 1.21 | 1.34 |
| 3 | E | 81 | VAL | C-N | -5.34 | 1.21 | 1.34 |
| 3 | y | 81 | VAL | C-N | -5.33 | 1.21 | 1.34 |
| 3 | EE | 81 | VAL | C-N | -5.31 | 1.21 | 1.34 |

All (226) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | BF | 186 | ARG | NE-CZ-NH1 | -11.68 | 114.46 | 120.30 |
| 11 | s | 186 | ARG | NE-CZ-NH1 | -11.58 | 114.51 | 120.30 |
| 11 | GB | 186 | ARG | NE-CZ-NH1 | -11.56 | 114.52 | 120.30 |
| 11 | V | 186 | ARG | NE-CZ-NH1 | -11.54 | 114.53 | 120.30 |
| 11 | DI | 186 | ARG | NE-CZ-NH1 | -11.50 | 114.55 | 120.30 |
| 11 | IE | 186 | ARG | NE-CZ-NH1 | -11.49 | 114.55 | 120.30 |
| 13 | YB | 75[A] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YB | 75[B] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YB | 75[C] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YB | 75[D] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YB | 75[E] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YB | 75[F] | GLY | C-N-CD | -9.24 | 100.28 | 120.60 |
| 13 | YA | 75[A] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YA | 75[B] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YA | 75[C] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YA | 75[D] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YA | 75[E] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YA | 75[F] | GLY | C-N-CD | -9.23 | 100.30 | 120.60 |
| 13 | YC | 75[A] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 13 | YC | 75[B] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 13 | YC | 75[C] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 13 | YC | 75[D] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 13 | YC | 75[E] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 13 | YC | 75[F] | GLY | C-N-CD | -9.21 | 100.33 | 120.60 |
| 11 | GB | 186 | ARG | NE-CZ-NH2 | 8.27 | 124.43 | 120.30 |
| 11 | BF | 186 | ARG | NE-CZ-NH2 | 8.22 | 124.41 | 120.30 |
| 11 | V | 186 | ARG | NE-CZ-NH2 | 8.18 | 124.39 | 120.30 |
| 11 | IE | 186 | ARG | NE-CZ-NH2 | 8.13 | 124.37 | 120.30 |
| 11 | DI | 186 | ARG | NE-CZ-NH2 | 8.11 | 124.36 | 120.30 |
| 11 | s | 186 | ARG | NE-CZ-NH2 | 8.08 | 124.34 | 120.30 |
| 12 | BG | 231 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 12 | W | 231 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 12 | GC | 231 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 5 | CG | 285 | LEU | CB-CG-CD1 | -6.42 | 100.09 | 111.00 |
| 12 | IF | 231 | ASP | CB-CG-OD1 | 6.41 | 124.07 | 118.30 |
| 12 | t | 231 | ASP | CB-CG-OD1 | 6.41 | 124.07 | 118.30 |
| 12 | DJ | 231 | ASP | CB-CG-OD1 | 6.41 | 124.07 | 118.30 |
| 5 | g | 285 | LEU | CB-CG-CD1 | -6.40 | 100.12 | 111.00 |
| 5 | EJ | 285 | LEU | CB-CG-CD1 | -6.39 | 100.14 | 111.00 |
| 5 | h | 326 | MET | CG-SD-CE | -6.37 | 90.00 | 100.20 |
| 5 | K | 326 | MET | CG-SD-CE | -6.37 | 90.01 | 100.20 |
| 5 | AD | 285 | LEU | CB-CG-CD1 | -6.37 | 100.17 | 111.00 |
| 5 | HC | 285 | LEU | CB-CG-CD1 | -6.37 | 100.17 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | J | 285 | LEU | CB-CG-CD1 | -6.37 | 100.17 | 111.00 |
| 5 | AE | 326 | MET | CG-SD-CE | -6.36 | 90.02 | 100.20 |
| 5 | FA | 326 | MET | CG-SD-CE | -6.35 | 90.04 | 100.20 |
| 5 | HD | 326 | MET | CG-SD-CE | -6.35 | 90.04 | 100.20 |
| 5 | CH | 326 | MET | CG-SD-CE | -6.35 | 90.05 | 100.20 |
| 10 | GA | 286 | VAL | CB-CA-C | 6.11 | 123.00 | 111.40 |
| 10 | BE | 286 | VAL | CB-CA-C | 6.10 | 122.99 | 111.40 |
| 5 | EJ | 326 | MET | CG-SD-CE | -6.10 | 90.44 | 100.20 |
| 10 | r | 286 | VAL | CB-CA-C | 6.10 | 122.98 | 111.40 |
| 10 | U | 286 | VAL | CB-CA-C | 6.09 | 122.98 | 111.40 |
| 5 | HC | 326 | MET | CG-SD-CE | -6.09 | 90.45 | 100.20 |
| 5 | AD | 326 | MET | CG-SD-CE | -6.09 | 90.46 | 100.20 |
| 5 | CG | 326 | MET | CG-SD-CE | -6.09 | 90.46 | 100.20 |
| 5 | J | 326 | MET | CG-SD-CE | -6.08 | 90.47 | 100.20 |
| 5 | g | 326 | MET | CG-SD-CE | -6.08 | 90.47 | 100.20 |
| 10 | DH | 286 | VAL | CB-CA-C | 6.08 | 122.94 | 111.40 |
| 10 | ID | 286 | VAL | CB-CA-C | 6.06 | 122.92 | 111.40 |
| 5 | J | 301 | GLY | N-CA-C | -6.04 | 98.01 | 113.10 |
| 5 | AD | 301 | GLY | N-CA-C | -6.04 | 98.00 | 113.10 |
| 13 | YA | 34[A] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 13 | YA | 34[B] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 13 | YA | 34[C] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 13 | YA | 34[D] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 13 | YA | 34[E] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 13 | YA | 34[F] | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 5 | g | 301 | GLY | N-CA-C | -6.04 | 98.01 | 113.10 |
| 5 | HC | 301 | GLY | N-CA-C | -6.03 | 98.03 | 113.10 |
| 5 | EJ | 301 | GLY | N-CA-C | -6.02 | 98.04 | 113.10 |
| 5 | CG | 301 | GLY | N-CA-C | -6.02 | 98.04 | 113.10 |
| 13 | YB | 34[A] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YB | 34[B] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YB | 34[C] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YB | 34[D] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YB | 34[E] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YB | 34[F] | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 13 | YC | 34[A] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 13 | YC | 34[B] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 13 | YC | 34[C] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 13 | YC | 34[D] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 13 | YC | 34[E] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 13 | YC | 34[F] | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 10 | U | 287 | VAL | CG1-CB-CG2 | -5.99 | 101.32 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | ID | 287 | VAL | CG1-CB-CG2 | -5.98 | 101.34 | 110.90 |
| 10 | r | 287 | VAL | CG1-CB-CG2 | -5.97 | 101.35 | 110.90 |
| 10 | BE | 287 | VAL | CG1-CB-CG2 | -5.97 | 101.35 | 110.90 |
| 10 | GA | 287 | VAL | CG1-CB-CG2 | -5.97 | 101.35 | 110.90 |
| 10 | DH | 287 | VAL | CG1-CB-CG2 | -5.96 | 101.36 | 110.90 |
| 1 | GE | 60 | LEU | CA-CB-CG | -5.96 | 101.59 | 115.30 |
| 1 | BI | 60 | LEU | CA-CB-CG | -5.94 | 101.63 | 115.30 |
| 1 | v | 60 | LEU | CA-CB-CG | -5.94 | 101.64 | 115.30 |
| 1 | EB | 60 | LEU | CA-CB-CG | -5.94 | 101.64 | 115.30 |
| 1 | B | 60 | LEU | CA-CB-CG | -5.93 | 101.67 | 115.30 |
| 1 | Y | 60 | LEU | CA-CB-CG | -5.92 | 101.69 | 115.30 |
| 2 | EC | 715 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |
| 2 | BJ | 715 | LEU | CA-CB-CG | 5.75 | 128.54 | 115.30 |
| 5 | AC | 326 | MET | CG-SD-CE | -5.75 | 91.00 | 100.20 |
| 2 | w | 715 | LEU | CA-CB-CG | 5.75 | 128.51 | 115.30 |
| 2 | C | 715 | LEU | CA-CB-CG | 5.74 | 128.50 | 115.30 |
| 5 | EI | 326 | MET | CG-SD-CE | -5.74 | 91.02 | 100.20 |
| 2 | Z | 715 | LEU | CA-CB-CG | 5.73 | 128.49 | 115.30 |
| 2 | GF | 715 | LEU | CA-CB-CG | 5.73 | 128.47 | 115.30 |
| 5 | f | 326 | MET | CG-SD-CE | -5.72 | 91.04 | 100.20 |
| 5 | HB | 326 | MET | CG-SD-CE | -5.72 | 91.04 | 100.20 |
| 5 | CF | 326 | MET | CG-SD-CE | -5.72 | 91.05 | 100.20 |
| 2 | w | 965 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |
| 5 | I | 326 | MET | CG-SD-CE | -5.72 | 91.05 | 100.20 |
| 5 | AD | 365 | ILE | C-N-CD | 5.71 | 140.40 | 128.40 |
| 5 | EJ | 365 | ILE | C-N-CD | 5.71 | 140.40 | 128.40 |
| 5 | g | 365 | ILE | C-N-CD | 5.70 | 140.38 | 128.40 |
| 5 | HC | 365 | ILE | C-N-CD | 5.70 | 140.37 | 128.40 |
| 5 | J | 365 | ILE | C-N-CD | 5.70 | 140.37 | 128.40 |
| 5 | CG | 365 | ILE | C-N-CD | 5.70 | 140.37 | 128.40 |
| 2 | C | 965 | LEU | CA-CB-CG | 5.70 | 128.41 | 115.30 |
| 2 | EC | 965 | LEU | CA-CB-CG | 5.69 | 128.39 | 115.30 |
| 2 | Z | 965 | LEU | CA-CB-CG | 5.69 | 128.38 | 115.30 |
| 2 | GF | 965 | LEU | CA-CB-CG | 5.69 | 128.38 | 115.30 |
| 2 | BJ | 965 | LEU | CA-CB-CG | 5.68 | 128.37 | 115.30 |
| 5 | HD | 337 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 12 | t | 191 | LEU | CA-CB-CG | -5.46 | 102.75 | 115.30 |
| 5 | K | 337 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 12 | IF | 191 | LEU | CA-CB-CG | -5.45 | 102.76 | 115.30 |
| 5 | h | 337 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 12 | W | 191 | LEU | CA-CB-CG | -5.44 | 102.79 | 115.30 |
| 5 | I | 406 | LEU | CA-CB-CG | -5.43 | 102.80 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | GC | 191 | LEU | CA-CB-CG | -5.43 | 102.80 | 115.30 |
| 12 | DJ | 191 | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[A] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[B] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[C] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[D] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[E] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 14 | YF | 259[F] | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 5 | EI | 406 | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 5 | CF | 406 | LEU | CA-CB-CG | -5.43 | 102.82 | 115.30 |
| 5 | CH | 337 | ASP | CB-CG-OD1 | 5.42 | 123.18 | 118.30 |
| 5 | AC | 406 | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YD | 259[A] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YD | 259[B] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YD | 259[C] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YD | 259[D] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YD | 259[E] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YD | 259[F] | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 14 | YE | 259[A] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YE | 259[B] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YE | 259[C] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YE | 259[D] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YE | 259[E] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 14 | YE | 259[F] | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 5 | HB | 406 | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 1 | GD | 527 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | A | 527 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 12 | BG | 191 | LEU | CA-CB-CG | -5.41 | 102.87 | 115.30 |
| 1 | u | 527 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 5 | AE | 337 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | BH | 527 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 5 | f | 406 | LEU | CA-CB-CG | -5.40 | 102.88 | 115.30 |
| 5 | FA | 337 | ASP | CB-CG-OD1 | 5.39 | 123.16 | 118.30 |
| 1 | X | 527 | ASP | CB-CG-OD1 | 5.38 | 123.15 | 118.30 |
| 1 | EA | 527 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 5 | AD | 62 | ALA | N-CA-C | 5.34 | 125.41 | 111.00 |
| 5 | g | 62 | ALA | N-CA-C | 5.33 | 125.40 | 111.00 |
| 5 | EJ | 62 | ALA | N-CA-C | 5.33 | 125.40 | 111.00 |
| 5 | CG | 62 | ALA | N-CA-C | 5.33 | 125.40 | 111.00 |
| 11 | V | 2 | LEU | CB-CG-CD1 | -5.33 | 101.94 | 111.00 |
| 12 | DJ | 163 | ARG | NE-CZ-NH2 | 5.32 | 122.96 | 120.30 |
| 5 | HC | 62 | ALA | N-CA-C | 5.32 | 125.36 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | DI | 2 | LEU | CB-CG-CD1 | -5.32 | 101.96 | 111.00 |
| 5 | J | 62 | ALA | N-CA-C | 5.31 | 125.35 | 111.00 |
| 11 | BF | 2 | LEU | CB-CG-CD1 | -5.31 | 101.97 | 111.00 |
| 11 | IE | 2 | LEU | CB-CG-CD1 | -5.31 | 101.98 | 111.00 |
| 11 | s | 2 | LEU | CB-CG-CD1 | -5.30 | 101.99 | 111.00 |
| 11 | GB | 2 | LEU | CB-CG-CD1 | -5.29 | 102.00 | 111.00 |
| 13 | YB | 75[A] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YB | 75[B] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YB | 75[C] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YB | 75[D] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YB | 75[E] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YB | 75[F] | GLY | C-N-CA | 5.27 | 144.15 | 122.00 |
| 13 | YA | 75[A] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YA | 75[B] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YA | 75[C] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YA | 75[D] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YA | 75[E] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YA | 75[F] | GLY | C-N-CA | 5.27 | 144.14 | 122.00 |
| 13 | YC | 75[A] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 13 | YC | 75[B] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 13 | YC | 75[C] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 13 | YC | 75[D] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 13 | YC | 75[E] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 13 | YC | 75[F] | GLY | C-N-CA | 5.26 | 144.11 | 122.00 |
| 12 | IF | 163 | ARG | NE-CZ-NH2 | 5.25 | 122.93 | 120.30 |
| 12 | t | 163 | ARG | NE-CZ-NH2 | 5.23 | 122.91 | 120.30 |
| 12 | W | 163 | ARG | NE-CZ-NH2 | 5.17 | 122.89 | 120.30 |
| 12 | BG | 163 | ARG | NE-CZ-NH2 | 5.15 | 122.88 | 120.30 |
| 13 | YA | 8[A] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YA | 8[B] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YA | 8[C] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YA | 8[D] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YA | 8[E] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YA | 8[F] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[A] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[B] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[C] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[D] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[E] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YC | 8[F] | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 13 | YB | 8[A] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |
| 13 | YB | 8[B] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | YB | 8[C] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |
| 13 | YB | 8[D] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |
| 13 | YB | 8[E] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |
| 13 | YB | 8[F] | LEU | CA-CB-CG | -5.14 | 103.47 | 115.30 |
| 12 | GC | 163 | ARG | NE-CZ-NH2 | 5.11 | 122.86 | 120.30 |
| 5 | AE | 556 | GLN | N-CA-CB | 5.07 | 119.72 | 110.60 |
| 5 | HD | 556 | GLN | N-CA-CB | 5.07 | 119.72 | 110.60 |
| 5 | CH | 556 | GLN | N-CA-CB | 5.06 | 119.72 | 110.60 |
| 5 | K | 556 | GLN | N-CA-CB | 5.06 | 119.70 | 110.60 |
| 5 | h | 556 | GLN | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 5 | FA | 556 | GLN | N-CA-CB | 5.04 | 119.66 | 110.60 |
| 12 | DJ | 163 | ARG | NE-CZ-NH1 | -5.03 | 117.78 | 120.30 |
| 5 | h | 62 | ALA | N-CA-C | 5.02 | 124.55 | 111.00 |
| 5 | K | 62 | ALA | N-CA-C | 5.01 | 124.53 | 111.00 |
| 5 | HD | 62 | ALA | N-CA-C | 5.00 | 124.51 | 111.00 |

There are no chirality outliers.

All (783) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 313 | ALA | Peptide |
| 5 | AC | 100 | ALA | Peptide |
| 5 | AC | 102 | TRP | Peptide |
| 5 | AC | 127 | ASN | Peptide |
| 5 | AC | 155 | THR | Peptide |
| 5 | AC | 196 | ARG | Peptide |
| 5 | AC | 267 | ASP | Peptide |
| 5 | AC | 276 | LEU | Peptide |
| 5 | AC | 278 | GLY | Peptide |
| 5 | AC | 293 | PHE | Peptide |
| 5 | AC | 333 | GLY | Peptide |
| 5 | AC | 364 | GLY | Peptide |
| 5 | AC | 365 | ILE | Peptide |
| 5 | AC | 366 | PRO | Peptide |
| 5 | AC | 555 | CYS | Peptide |
| 5 | AC | 61 | THR | Peptide |
| 5 | AC | 84 | GLY | Peptide |
| 5 | AC | 9 | ASN | Peptide |
| 5 | AD | 100 | ALA | Peptide |
| 5 | AD | 102 | TRP | Peptide |
| 5 | AD | 150 | GLN | Peptide |
| 5 | AD | 152 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | AD | 196 | ARG | Peptide |
| 5 | AD | 215 | PRO | Peptide |
| 5 | AD | 278 | GLY | Peptide |
| 5 | AD | 293 | PHE | Peptide |
| 5 | AD | 300 | PRO | Peptide |
| 5 | AD | 302 | GLU | Peptide |
| 5 | AD | 333 | GLY | Peptide |
| 5 | AD | 61 | THR | Peptide |
| 5 | AD | 84 | GLY | Peptide |
| 5 | AE | 100 | ALA | Peptide |
| 5 | AE | 102 | TRP | Peptide |
| 5 | AE | 127 | ASN | Peptide |
| 5 | AE | 151 | ILE | Peptide |
| 5 | AE | 156 | SER | Peptide |
| 5 | AE | 196 | ARG | Peptide |
| 5 | AE | 215 | PRO | Peptide |
| 5 | AE | 256 | SER | Peptide |
| 5 | AE | 276 | LEU | Peptide |
| 5 | AE | 293 | PHE | Peptide |
| 5 | AE | 320 | LEU | Peptide |
| 5 | AE | 333 | GLY | Peptide |
| 5 | AE | 361 | ASP | Peptide |
| 5 | AE | 391 | GLY | Peptide |
| 5 | AE | 61 | THR | Peptide |
| 5 | AE | 84 | GLY | Peptide |
| 6 | AF | 11 | ILE | Peptide |
| 6 | AF | 8 | ALA | Peptide |
| 6 | AF | 9 | GLY | Peptide |
| 6 | AG | 11 | ILE | Peptide |
| 6 | AG | 8 | ALA | Peptide |
| 6 | AG | 9 | GLY | Peptide |
| 6 | AH | 11 | ILE | Peptide |
| 6 | AH | 8 | ALA | Peptide |
| 6 | AH | 9 | GLY | Peptide |
| 7 | AI | 28 | GLU | Peptide |
| 7 | AI | 44 | VAL | Peptide |
| 7 | AI | 46 | GLY | Peptide |
| 7 | AI | 47 | VAL | Peptide |
| 7 | AJ | 152 | ALA | Peptide |
| 7 | AJ | 178 | PRO | Peptide |
| 7 | AJ | 28 | GLU | Peptide |
| 7 | AJ | 46 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | AJ | 47 | VAL | Peptide |
| 7 | AJ | 87 | TYR | Peptide |
| 1 | B | 136 | LYS | Peptide |
| 1 | B | 137 | ASP | Peptide |
| 1 | B | 18 | PRO | Peptide |
| 1 | B | 182 | LEU | Peptide |
| 1 | B | 20 | ILE | Peptide |
| 1 | B | 218 | GLY | Peptide |
| 1 | B | 256 | TYR | Peptide |
| 1 | B | 533 | ASP | Peptide |
| 7 | BA | 152 | ALA | Peptide |
| 7 | BA | 28 | GLU | Peptide |
| 7 | BA | 47 | VAL | Peptide |
| 7 | BA | 57 | ILE | Peptide |
| 7 | BA | 86 | SER | Peptide |
| 10 | BE | 340 | SER | Peptide |
| 11 | BF | 2 | LEU | Peptide |
| 1 | BH | 313 | ALA | Peptide |
| 1 | BI | 136 | LYS | Peptide |
| 1 | BI | 137 | ASP | Peptide |
| 1 | BI | 18 | PRO | Peptide |
| 1 | BI | 182 | LEU | Peptide |
| 1 | BI | 20 | ILE | Peptide |
| 1 | BI | 218 | GLY | Peptide |
| 1 | BI | 256 | TYR | Peptide |
| 1 | BI | 533 | ASP | Peptide |
| 2 | BJ | 105 | THR | Peptide |
| 2 | BJ | 134 | TYR | Peptide |
| 2 | BJ | 136 | ASN | Peptide |
| 2 | BJ | 156 | SER | Peptide |
| 2 | BJ | 167 | ILE | Peptide |
| 2 | BJ | 215 | LYS | Peptide |
| 2 | BJ | 227 | ASP | Peptide |
| 2 | BJ | 235 | LYS | Peptide |
| 2 | BJ | 298 | ALA | Peptide |
| 2 | BJ | 332 | SER | Peptide |
| 2 | BJ | 339 | ASP | Peptide |
| 2 | BJ | 342 | SER | Peptide |
| 2 | BJ | 343 | PRO | Peptide |
| 2 | BJ | 348 | ARG | Peptide |
| 2 | BJ | 353 | ASP | Peptide |
| 2 | BJ | 398 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | BJ | 409 | ASP | Peptide |
| 2 | BJ | 436 | THR | Peptide |
| 2 | BJ | 456 | VAL | Peptide |
| 2 | BJ | 508 | TYR | Peptide |
| 2 | BJ | 554 | ASP | Peptide |
| 2 | BJ | 600 | PHE | Peptide |
| 2 | BJ | 623 | LEU | Peptide |
| 2 | BJ | 624 | GLN | Peptide |
| 2 | BJ | 625 | ASN | Peptide |
| 2 | BJ | 706 | SER | Peptide |
| 2 | BJ | 824 | GLN | Peptide |
| 2 | BJ | 850 | ASN | Peptide |
| 2 | BJ | 920 | LYS | Peptide |
| 2 | BJ | 925 | LEU | Peptide |
| 2 | BJ | 929 | TYR | Peptide |
| 2 | BJ | 940 | GLY | Peptide |
| 2 | BJ | 965 | LEU | Peptide |
| 2 | BJ | 967 | ASP | Peptide |
| 2 | BJ | 984 | SER | Peptide |
| 2 | BJ | 988 | LYS | Peptide |
| 2 | BJ | 989 | LEU | Peptide |
| 2 | BJ | 991 | SER | Peptide |
| 2 | C | 105 | THR | Peptide |
| 2 | C | 134 | TYR | Peptide |
| 2 | C | 136 | ASN | Peptide |
| 2 | C | 156 | SER | Peptide |
| 2 | C | 167 | ILE | Peptide |
| 2 | C | 215 | LYS | Peptide |
| 2 | C | 227 | ASP | Peptide |
| 2 | C | 235 | LYS | Peptide |
| 2 | C | 298 | ALA | Peptide |
| 2 | C | 332 | SER | Peptide |
| 2 | C | 339 | ASP | Peptide |
| 2 | C | 342 | SER | Peptide |
| 2 | C | 343 | PRO | Peptide |
| 2 | C | 348 | ARG | Peptide |
| 2 | C | 353 | ASP | Peptide |
| 2 | C | 398 | SER | Peptide |
| 2 | C | 409 | ASP | Peptide |
| 2 | C | 436 | THR | Peptide |
| 2 | C | 456 | VAL | Peptide |
| 2 | C | 508 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | C | 554 | ASP | Peptide |
| 2 | C | 600 | PHE | Peptide |
| 2 | C | 623 | LEU | Peptide |
| 2 | C | 624 | GLN | Peptide |
| 2 | C | 625 | ASN | Peptide |
| 2 | C | 706 | SER | Peptide |
| 2 | C | 824 | GLN | Peptide |
| 2 | C | 850 | ASN | Peptide |
| 2 | C | 920 | LYS | Peptide |
| 2 | C | 925 | LEU | Peptide |
| 2 | C | 929 | TYR | Peptide |
| 2 | C | 940 | GLY | Peptide |
| 2 | C | 965 | LEU | Peptide |
| 2 | C | 967 | ASP | Peptide |
| 2 | C | 984 | SER | Peptide |
| 2 | C | 988 | LYS | Peptide |
| 2 | C | 989 | LEU | Peptide |
| 2 | C | 991 | SER | Peptide |
| 3 | CA | 102 | ASP | Peptide |
| 3 | CA | 262 | ALA | Peptide |
| 3 | CB | 177 | GLU | Peptide |
| 3 | CB | 228 | ASN | Peptide |
| 3 | CB | 32 | PRO | Peptide |
| 5 | CF | 100 | ALA | Peptide |
| 5 | CF | 102 | TRP | Peptide |
| 5 | CF | 127 | ASN | Peptide |
| 5 | CF | 155 | THR | Peptide |
| 5 | CF | 196 | ARG | Peptide |
| 5 | CF | 267 | ASP | Peptide |
| 5 | CF | 276 | LEU | Peptide |
| 5 | CF | 278 | GLY | Peptide |
| 5 | CF | 293 | PHE | Peptide |
| 5 | CF | 333 | GLY | Peptide |
| 5 | CF | 364 | GLY | Peptide |
| 5 | CF | 365 | ILE | Peptide |
| 5 | CF | 366 | PRO | Peptide |
| 5 | CF | 555 | CYS | Peptide |
| 5 | CF | 61 | THR | Peptide |
| 5 | CF | 84 | GLY | Peptide |
| 5 | CF | 9 | ASN | Peptide |
| 5 | CG | 100 | ALA | Peptide |
| 5 | CG | 102 | TRP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | CG | 150 | GLN | Peptide |
| 5 | CG | 152 | ASP | Peptide |
| 5 | CG | 196 | ARG | Peptide |
| 5 | CG | 215 | PRO | Peptide |
| 5 | CG | 278 | GLY | Peptide |
| 5 | CG | 293 | PHE | Peptide |
| 5 | CG | 300 | PRO | Peptide |
| 5 | CG | 302 | GLU | Peptide |
| 5 | CG | 333 | GLY | Peptide |
| 5 | CG | 61 | THR | Peptide |
| 5 | CG | 84 | GLY | Peptide |
| 5 | CH | 100 | ALA | Peptide |
| 5 | CH | 102 | TRP | Peptide |
| 5 | CH | 127 | ASN | Peptide |
| 5 | CH | 151 | ILE | Peptide |
| 5 | CH | 156 | SER | Peptide |
| 5 | CH | 196 | ARG | Peptide |
| 5 | CH | 215 | PRO | Peptide |
| 5 | CH | 256 | SER | Peptide |
| 5 | CH | 276 | LEU | Peptide |
| 5 | CH | 293 | PHE | Peptide |
| 5 | CH | 320 | LEU | Peptide |
| 5 | CH | 333 | GLY | Peptide |
| 5 | CH | 361 | ASP | Peptide |
| 5 | CH | 391 | GLY | Peptide |
| 5 | CH | 61 | THR | Peptide |
| 5 | CH | 84 | GLY | Peptide |
| 6 | CI | 11 | ILE | Peptide |
| 6 | CI | 8 | ALA | Peptide |
| 6 | CI | 9 | GLY | Peptide |
| 6 | CJ | 11 | ILE | Peptide |
| 6 | CJ | 8 | ALA | Peptide |
| 6 | CJ | 9 | GLY | Peptide |
| 3 | D | 102 | ASP | Peptide |
| 3 | D | 262 | ALA | Peptide |
| 6 | DA | 11 | ILE | Peptide |
| 6 | DA | 8 | ALA | Peptide |
| 6 | DA | 9 | GLY | Peptide |
| 7 | DB | 28 | GLU | Peptide |
| 7 | DB | 44 | VAL | Peptide |
| 7 | DB | 46 | GLY | Peptide |
| 7 | DB | 47 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | DC | 152 | ALA | Peptide |
| 7 | DC | 178 | PRO | Peptide |
| 7 | DC | 28 | GLU | Peptide |
| 7 | DC | 46 | GLY | Peptide |
| 7 | DC | 47 | VAL | Peptide |
| 7 | DC | 87 | TYR | Peptide |
| 7 | DD | 152 | ALA | Peptide |
| 7 | DD | 28 | GLU | Peptide |
| 7 | DD | 47 | VAL | Peptide |
| 7 | DD | 57 | ILE | Peptide |
| 7 | DD | 86 | SER | Peptide |
| 10 | DH | 340 | SER | Peptide |
| 11 | DI | 2 | LEU | Peptide |
| 3 | E | 177 | GLU | Peptide |
| 3 | E | 228 | ASN | Peptide |
| 3 | E | 32 | PRO | Peptide |
| 1 | EA | 313 | ALA | Peptide |
| 1 | EB | 136 | LYS | Peptide |
| 1 | EB | 137 | ASP | Peptide |
| 1 | EB | 18 | PRO | Peptide |
| 1 | EB | 182 | LEU | Peptide |
| 1 | EB | 20 | ILE | Peptide |
| 1 | EB | 218 | GLY | Peptide |
| 1 | EB | 256 | TYR | Peptide |
| 1 | EB | 533 | ASP | Peptide |
| 2 | EC | 105 | THR | Peptide |
| 2 | EC | 134 | TYR | Peptide |
| 2 | EC | 136 | ASN | Peptide |
| 2 | EC | 156 | SER | Peptide |
| 2 | EC | 167 | ILE | Peptide |
| 2 | EC | 215 | LYS | Peptide |
| 2 | EC | 227 | ASP | Peptide |
| 2 | EC | 235 | LYS | Peptide |
| 2 | EC | 298 | ALA | Peptide |
| 2 | EC | 332 | SER | Peptide |
| 2 | EC | 339 | ASP | Peptide |
| 2 | EC | 342 | SER | Peptide |
| 2 | EC | 343 | PRO | Peptide |
| 2 | EC | 348 | ARG | Peptide |
| 2 | EC | 353 | ASP | Peptide |
| 2 | EC | 398 | SER | Peptide |
| 2 | EC | 409 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | EC | 436 | THR | Peptide |
| 2 | EC | 456 | VAL | Peptide |
| 2 | EC | 508 | TYR | Peptide |
| 2 | EC | 554 | ASP | Peptide |
| 2 | EC | 600 | PHE | Peptide |
| 2 | EC | 623 | LEU | Peptide |
| 2 | EC | 624 | GLN | Peptide |
| 2 | EC | 625 | ASN | Peptide |
| 2 | EC | 706 | SER | Peptide |
| 2 | EC | 824 | GLN | Peptide |
| 2 | EC | 850 | ASN | Peptide |
| 2 | EC | 920 | LYS | Peptide |
| 2 | EC | 925 | LEU | Peptide |
| 2 | EC | 929 | TYR | Peptide |
| 2 | EC | 940 | GLY | Peptide |
| 2 | EC | 965 | LEU | Peptide |
| 2 | EC | 967 | ASP | Peptide |
| 2 | EC | 984 | SER | Peptide |
| 2 | EC | 988 | LYS | Peptide |
| 2 | EC | 989 | LEU | Peptide |
| 2 | EC | 991 | SER | Peptide |
| 3 | ED | 102 | ASP | Peptide |
| 3 | ED | 262 | ALA | Peptide |
| 3 | EE | 177 | GLU | Peptide |
| 3 | EE | 228 | ASN | Peptide |
| 3 | EE | 32 | PRO | Peptide |
| 5 | EI | 100 | ALA | Peptide |
| 5 | EI | 102 | TRP | Peptide |
| 5 | EI | 127 | ASN | Peptide |
| 5 | EI | 155 | THR | Peptide |
| 5 | EI | 196 | ARG | Peptide |
| 5 | EI | 267 | ASP | Peptide |
| 5 | EI | 276 | LEU | Peptide |
| 5 | EI | 278 | GLY | Peptide |
| 5 | EI | 293 | PHE | Peptide |
| 5 | EI | 333 | GLY | Peptide |
| 5 | EI | 364 | GLY | Peptide |
| 5 | EI | 365 | ILE | Peptide |
| 5 | EI | 366 | PRO | Peptide |
| 5 | EI | 555 | CYS | Peptide |
| 5 | EI | 61 | THR | Peptide |
| 5 | EI | 84 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | EI | 9 | ASN | Peptide |
| 5 | EJ | 100 | ALA | Peptide |
| 5 | EJ | 102 | TRP | Peptide |
| 5 | EJ | 150 | GLN | Peptide |
| 5 | EJ | 152 | ASP | Peptide |
| 5 | EJ | 196 | ARG | Peptide |
| 5 | EJ | 215 | PRO | Peptide |
| 5 | EJ | 278 | GLY | Peptide |
| 5 | EJ | 293 | PHE | Peptide |
| 5 | EJ | 300 | PRO | Peptide |
| 5 | EJ | 302 | GLU | Peptide |
| 5 | EJ | 333 | GLY | Peptide |
| 5 | EJ | 61 | THR | Peptide |
| 5 | EJ | 84 | GLY | Peptide |
| 5 | FA | 100 | ALA | Peptide |
| 5 | FA | 102 | TRP | Peptide |
| 5 | FA | 127 | ASN | Peptide |
| 5 | FA | 151 | ILE | Peptide |
| 5 | FA | 156 | SER | Peptide |
| 5 | FA | 196 | ARG | Peptide |
| 5 | FA | 215 | PRO | Peptide |
| 5 | FA | 256 | SER | Peptide |
| 5 | FA | 276 | LEU | Peptide |
| 5 | FA | 293 | PHE | Peptide |
| 5 | FA | 320 | LEU | Peptide |
| 5 | FA | 333 | GLY | Peptide |
| 5 | FA | 361 | ASP | Peptide |
| 5 | FA | 391 | GLY | Peptide |
| 5 | FA | 61 | THR | Peptide |
| 5 | FA | 84 | GLY | Peptide |
| 6 | FB | 11 | ILE | Peptide |
| 6 | FB | 8 | ALA | Peptide |
| 6 | FB | 9 | GLY | Peptide |
| 6 | FC | 11 | ILE | Peptide |
| 6 | FC | 8 | ALA | Peptide |
| 6 | FC | 9 | GLY | Peptide |
| 6 | FD | 11 | ILE | Peptide |
| 6 | FD | 8 | ALA | Peptide |
| 6 | FD | 9 | GLY | Peptide |
| 7 | FE | 28 | GLU | Peptide |
| 7 | FE | 44 | VAL | Peptide |
| 7 | FE | 46 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | FE | 47 | VAL | Peptide |
| 7 | FF | 152 | ALA | Peptide |
| 7 | FF | 178 | PRO | Peptide |
| 7 | FF | 28 | GLU | Peptide |
| 7 | FF | 46 | GLY | Peptide |
| 7 | FF | 47 | VAL | Peptide |
| 7 | FF | 87 | TYR | Peptide |
| 7 | FG | 152 | ALA | Peptide |
| 7 | FG | 28 | GLU | Peptide |
| 7 | FG | 47 | VAL | Peptide |
| 7 | FG | 57 | ILE | Peptide |
| 7 | FG | 86 | SER | Peptide |
| 10 | GA | 340 | SER | Peptide |
| 11 | GB | 2 | LEU | Peptide |
| 1 | GD | 313 | ALA | Peptide |
| 1 | GE | 136 | LYS | Peptide |
| 1 | GE | 137 | ASP | Peptide |
| 1 | GE | 18 | PRO | Peptide |
| 1 | GE | 182 | LEU | Peptide |
| 1 | GE | 20 | ILE | Peptide |
| 1 | GE | 218 | GLY | Peptide |
| 1 | GE | 256 | TYR | Peptide |
| 1 | GE | 533 | ASP | Peptide |
| 2 | GF | 105 | THR | Peptide |
| 2 | GF | 134 | TYR | Peptide |
| 2 | GF | 136 | ASN | Peptide |
| 2 | GF | 156 | SER | Peptide |
| 2 | GF | 167 | ILE | Peptide |
| 2 | GF | 215 | LYS | Peptide |
| 2 | GF | 227 | ASP | Peptide |
| 2 | GF | 235 | LYS | Peptide |
| 2 | GF | 298 | ALA | Peptide |
| 2 | GF | 332 | SER | Peptide |
| 2 | GF | 339 | ASP | Peptide |
| 2 | GF | 342 | SER | Peptide |
| 2 | GF | 343 | PRO | Peptide |
| 2 | GF | 348 | ARG | Peptide |
| 2 | GF | 353 | ASP | Peptide |
| 2 | GF | 398 | SER | Peptide |
| 2 | GF | 409 | ASP | Peptide |
| 2 | GF | 436 | THR | Peptide |
| 2 | GF | 456 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | GF | 508 | TYR | Peptide |
| 2 | GF | 554 | ASP | Peptide |
| 2 | GF | 600 | PHE | Peptide |
| 2 | GF | 623 | LEU | Peptide |
| 2 | GF | 624 | GLN | Peptide |
| 2 | GF | 625 | ASN | Peptide |
| 2 | GF | 706 | SER | Peptide |
| 2 | GF | 824 | GLN | Peptide |
| 2 | GF | 850 | ASN | Peptide |
| 2 | GF | 920 | LYS | Peptide |
| 2 | GF | 925 | LEU | Peptide |
| 2 | GF | 929 | TYR | Peptide |
| 2 | GF | 940 | GLY | Peptide |
| 2 | GF | 965 | LEU | Peptide |
| 2 | GF | 967 | ASP | Peptide |
| 2 | GF | 984 | SER | Peptide |
| 2 | GF | 988 | LYS | Peptide |
| 2 | GF | 989 | LEU | Peptide |
| 2 | GF | 991 | SER | Peptide |
| 3 | GG | 102 | ASP | Peptide |
| 3 | GG | 262 | ALA | Peptide |
| 3 | GH | 177 | GLU | Peptide |
| 3 | GH | 228 | ASN | Peptide |
| 3 | GH | 32 | PRO | Peptide |
| 5 | HB | 100 | ALA | Peptide |
| 5 | HB | 102 | TRP | Peptide |
| 5 | HB | 127 | ASN | Peptide |
| 5 | HB | 155 | THR | Peptide |
| 5 | HB | 196 | ARG | Peptide |
| 5 | HB | 267 | ASP | Peptide |
| 5 | HB | 276 | LEU | Peptide |
| 5 | HB | 278 | GLY | Peptide |
| 5 | HB | 293 | PHE | Peptide |
| 5 | HB | 333 | GLY | Peptide |
| 5 | HB | 364 | GLY | Peptide |
| 5 | HB | 365 | ILE | Peptide |
| 5 | HB | 366 | PRO | Peptide |
| 5 | HB | 555 | CYS | Peptide |
| 5 | HB | 61 | THR | Peptide |
| 5 | HB | 84 | GLY | Peptide |
| 5 | HB | 9 | ASN | Peptide |
| 5 | HC | 100 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | HC | 102 | TRP | Peptide |
| 5 | HC | 150 | GLN | Peptide |
| 5 | HC | 152 | ASP | Peptide |
| 5 | HC | 196 | ARG | Peptide |
| 5 | HC | 215 | PRO | Peptide |
| 5 | HC | 278 | GLY | Peptide |
| 5 | HC | 293 | PHE | Peptide |
| 5 | HC | 300 | PRO | Peptide |
| 5 | HC | 302 | GLU | Peptide |
| 5 | HC | 333 | GLY | Peptide |
| 5 | HC | 61 | THR | Peptide |
| 5 | HC | 84 | GLY | Peptide |
| 5 | HD | 100 | ALA | Peptide |
| 5 | HD | 102 | TRP | Peptide |
| 5 | HD | 127 | ASN | Peptide |
| 5 | HD | 151 | ILE | Peptide |
| 5 | HD | 156 | SER | Peptide |
| 5 | HD | 196 | ARG | Peptide |
| 5 | HD | 215 | PRO | Peptide |
| 5 | HD | 256 | SER | Peptide |
| 5 | HD | 276 | LEU | Peptide |
| 5 | HD | 293 | PHE | Peptide |
| 5 | HD | 320 | LEU | Peptide |
| 5 | HD | 333 | GLY | Peptide |
| 5 | HD | 361 | ASP | Peptide |
| 5 | HD | 391 | GLY | Peptide |
| 5 | HD | 61 | THR | Peptide |
| 5 | HD | 84 | GLY | Peptide |
| 6 | HE | 11 | ILE | Peptide |
| 6 | HE | 8 | ALA | Peptide |
| 6 | HE | 9 | GLY | Peptide |
| 6 | HF | 11 | ILE | Peptide |
| 6 | HF | 8 | ALA | Peptide |
| 6 | HF | 9 | GLY | Peptide |
| 6 | HG | 11 | ILE | Peptide |
| 6 | HG | 8 | ALA | Peptide |
| 6 | HG | 9 | GLY | Peptide |
| 7 | HH | 28 | GLU | Peptide |
| 7 | HH | 44 | VAL | Peptide |
| 7 | HH | 46 | GLY | Peptide |
| 7 | HH | 47 | VAL | Peptide |
| 7 | HI | 152 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | HI | 178 | PRO | Peptide |
| 7 | HI | 28 | GLU | Peptide |
| 7 | HI | 46 | GLY | Peptide |
| 7 | HI | 47 | VAL | Peptide |
| 7 | HI | 87 | TYR | Peptide |
| 7 | HJ | 152 | ALA | Peptide |
| 7 | HJ | 28 | GLU | Peptide |
| 7 | HJ | 47 | VAL | Peptide |
| 7 | HJ | 57 | ILE | Peptide |
| 7 | HJ | 86 | SER | Peptide |
| 5 | I | 100 | ALA | Peptide |
| 5 | I | 102 | TRP | Peptide |
| 5 | I | 127 | ASN | Peptide |
| 5 | I | 155 | THR | Peptide |
| 5 | I | 196 | ARG | Peptide |
| 5 | I | 267 | ASP | Peptide |
| 5 | I | 276 | LEU | Peptide |
| 5 | I | 278 | GLY | Peptide |
| 5 | I | 293 | PHE | Peptide |
| 5 | I | 333 | GLY | Peptide |
| 5 | I | 364 | GLY | Peptide |
| 5 | I | 365 | ILE | Peptide |
| 5 | I | 366 | PRO | Peptide |
| 5 | I | 555 | CYS | Peptide |
| 5 | I | 61 | THR | Peptide |
| 5 | I | 84 | GLY | Peptide |
| 5 | I | 9 | ASN | Peptide |
| 10 | ID | 340 | SER | Peptide |
| 11 | IE | 2 | LEU | Peptide |
| 5 | J | 100 | ALA | Peptide |
| 5 | J | 102 | TRP | Peptide |
| 5 | J | 150 | GLN | Peptide |
| 5 | J | 152 | ASP | Peptide |
| 5 | J | 196 | ARG | Peptide |
| 5 | J | 215 | PRO | Peptide |
| 5 | J | 278 | GLY | Peptide |
| 5 | J | 293 | PHE | Peptide |
| 5 | J | 300 | PRO | Peptide |
| 5 | J | 302 | GLU | Peptide |
| 5 | J | 333 | GLY | Peptide |
| 5 | J | 61 | THR | Peptide |
| 5 | J | 84 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | K | 100 | ALA | Peptide |
| 5 | K | 102 | TRP | Peptide |
| 5 | K | 127 | ASN | Peptide |
| 5 | K | 151 | ILE | Peptide |
| 5 | K | 156 | SER | Peptide |
| 5 | K | 196 | ARG | Peptide |
| 5 | K | 215 | PRO | Peptide |
| 5 | K | 256 | SER | Peptide |
| 5 | K | 276 | LEU | Peptide |
| 5 | K | 293 | PHE | Peptide |
| 5 | K | 320 | LEU | Peptide |
| 5 | K | 333 | GLY | Peptide |
| 5 | K | 361 | ASP | Peptide |
| 5 | K | 391 | GLY | Peptide |
| 5 | K | 61 | THR | Peptide |
| 5 | K | 84 | GLY | Peptide |
| 6 | L | 11 | ILE | Peptide |
| 6 | L | 8 | ALA | Peptide |
| 6 | L | 9 | GLY | Peptide |
| 6 | M | 11 | ILE | Peptide |
| 6 | M | 8 | ALA | Peptide |
| 6 | M | 9 | GLY | Peptide |
| 6 | N | 11 | ILE | Peptide |
| 6 | N | 8 | ALA | Peptide |
| 6 | N | 9 | GLY | Peptide |
| 7 | O | 28 | GLU | Peptide |
| 7 | O | 44 | VAL | Peptide |
| 7 | O | 46 | GLY | Peptide |
| 7 | O | 47 | VAL | Peptide |
| 7 | P | 152 | ALA | Peptide |
| 7 | P | 178 | PRO | Peptide |
| 7 | P | 28 | GLU | Peptide |
| 7 | P | 46 | GLY | Peptide |
| 7 | P | 47 | VAL | Peptide |
| 7 | P | 87 | TYR | Peptide |
| 7 | Q | 152 | ALA | Peptide |
| 7 | Q | 28 | GLU | Peptide |
| 7 | Q | 47 | VAL | Peptide |
| 7 | Q | 57 | ILE | Peptide |
| 7 | Q | 86 | SER | Peptide |
| 10 | U | 340 | SER | Peptide |
| 11 | V | 2 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | X | 313 | ALA | Peptide |
| 1 | Y | 136 | LYS | Peptide |
| 1 | Y | 137 | ASP | Peptide |
| 1 | Y | 18 | PRO | Peptide |
| 1 | Y | 182 | LEU | Peptide |
| 1 | Y | 20 | ILE | Peptide |
| 1 | Y | 218 | GLY | Peptide |
| 1 | Y | 256 | TYR | Peptide |
| 1 | Y | 533 | ASP | Peptide |
| 13 | YA | 74[A] | THR | Peptide |
| 13 | YA | 74[B] | THR | Peptide |
| 13 | YA | 74[C] | THR | Peptide |
| 13 | YA | 74[D] | THR | Peptide |
| 13 | YA | 74[E] | THR | Peptide |
| 13 | YA | 74[F] | THR | Peptide |
| 13 | YA | 75[B] | GLY | Peptide |
| 13 | YB | 74[A] | THR | Peptide |
| 13 | YB | 74[B] | THR | Peptide |
| 13 | YB | 74[C] | THR | Peptide |
| 13 | YB | 74[D] | THR | Peptide |
| 13 | YB | 74[E] | THR | Peptide |
| 13 | YB | 74[F] | THR | Peptide |
| 13 | YB | 75[B] | GLY | Peptide |
| 13 | YC | 74[A] | THR | Peptide |
| 13 | YC | 74[B] | THR | Peptide |
| 13 | YC | 74[C] | THR | Peptide |
| 13 | YC | 74[D] | THR | Peptide |
| 13 | YC | 74[E] | THR | Peptide |
| 13 | YC | 74[F] | THR | Peptide |
| 13 | YC | 75[B] | GLY | Peptide |
| 14 | YD | 366[A] | THR | Peptide |
| 14 | YD | 366[B] | THR | Peptide |
| 14 | YD | 366[C] | THR | Peptide |
| 14 | YD | 366[D] | THR | Peptide |
| 14 | YD | 366[E] | THR | Peptide |
| 14 | YD | 366[F] | THR | Peptide |
| 14 | YE | 366[A] | THR | Peptide |
| 14 | YE | 366[B] | THR | Peptide |
| 14 | YE | 366[C] | THR | Peptide |
| 14 | YE | 366[D] | THR | Peptide |
| 14 | YE | 366[E] | THR | Peptide |
| 14 | YE | 366[F] | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | YF | 366[A] | THR | Peptide |
| 14 | YF | 366[B] | THR | Peptide |
| 14 | YF | 366[C] | THR | Peptide |
| 14 | YF | 366[D] | THR | Peptide |
| 14 | YF | 366[E] | THR | Peptide |
| 14 | YF | 366[F] | THR | Peptide |
| 2 | Z | 105 | THR | Peptide |
| 2 | Z | 134 | TYR | Peptide |
| 2 | Z | 136 | ASN | Peptide |
| 2 | Z | 156 | SER | Peptide |
| 2 | Z | 167 | ILE | Peptide |
| 2 | Z | 215 | LYS | Peptide |
| 2 | Z | 227 | ASP | Peptide |
| 2 | Z | 235 | LYS | Peptide |
| 2 | Z | 298 | ALA | Peptide |
| 2 | Z | 332 | SER | Peptide |
| 2 | Z | 339 | ASP | Peptide |
| 2 | Z | 342 | SER | Peptide |
| 2 | Z | 343 | PRO | Peptide |
| 2 | Z | 348 | ARG | Peptide |
| 2 | Z | 353 | ASP | Peptide |
| 2 | Z | 398 | SER | Peptide |
| 2 | Z | 409 | ASP | Peptide |
| 2 | Z | 436 | THR | Peptide |
| 2 | Z | 456 | VAL | Peptide |
| 2 | Z | 508 | TYR | Peptide |
| 2 | Z | 554 | ASP | Peptide |
| 2 | Z | 600 | PHE | Peptide |
| 2 | Z | 623 | LEU | Peptide |
| 2 | Z | 624 | GLN | Peptide |
| 2 | Z | 625 | ASN | Peptide |
| 2 | Z | 706 | SER | Peptide |
| 2 | Z | 824 | GLN | Peptide |
| 2 | Z | 850 | ASN | Peptide |
| 2 | Z | 920 | LYS | Peptide |
| 2 | Z | 925 | LEU | Peptide |
| 2 | Z | 929 | TYR | Peptide |
| 2 | Z | 940 | GLY | Peptide |
| 2 | Z | 965 | LEU | Peptide |
| 2 | Z | 967 | ASP | Peptide |
| 2 | Z | 984 | SER | Peptide |
| 2 | Z | 988 | LYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | Z | 989 | LEU | Peptide |
| 2 | Z | 991 | SER | Peptide |
| 3 | a | 102 | ASP | Peptide |
| 3 | a | 262 | ALA | Peptide |
| 3 | b | 177 | GLU | Peptide |
| 3 | b | 228 | ASN | Peptide |
| 3 | b | 32 | PRO | Peptide |
| 5 | f | 100 | ALA | Peptide |
| 5 | f | 102 | TRP | Peptide |
| 5 | f | 127 | ASN | Peptide |
| 5 | f | 155 | THR | Peptide |
| 5 | f | 196 | ARG | Peptide |
| 5 | f | 267 | ASP | Peptide |
| 5 | f | 276 | LEU | Peptide |
| 5 | f | 278 | GLY | Peptide |
| 5 | f | 293 | PHE | Peptide |
| 5 | f | 333 | GLY | Peptide |
| 5 | f | 364 | GLY | Peptide |
| 5 | f | 365 | ILE | Peptide |
| 5 | f | 366 | PRO | Peptide |
| 5 | f | 555 | CYS | Peptide |
| 5 | f | 61 | THR | Peptide |
| 5 | f | 84 | GLY | Peptide |
| 5 | f | 9 | ASN | Peptide |
| 5 | g | 100 | ALA | Peptide |
| 5 | g | 102 | TRP | Peptide |
| 5 | g | 150 | GLN | Peptide |
| 5 | g | 152 | ASP | Peptide |
| 5 | g | 196 | ARG | Peptide |
| 5 | g | 215 | PRO | Peptide |
| 5 | g | 278 | GLY | Peptide |
| 5 | g | 293 | PHE | Peptide |
| 5 | g | 300 | PRO | Peptide |
| 5 | g | 302 | GLU | Peptide |
| 5 | g | 333 | GLY | Peptide |
| 5 | g | 61 | THR | Peptide |
| 5 | g | 84 | GLY | Peptide |
| 5 | h | 100 | ALA | Peptide |
| 5 | h | 102 | TRP | Peptide |
| 5 | h | 127 | ASN | Peptide |
| 5 | h | 151 | ILE | Peptide |
| 5 | h | 156 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | h | 196 | ARG | Peptide |
| 5 | h | 215 | PRO | Peptide |
| 5 | h | 256 | SER | Peptide |
| 5 | h | 276 | LEU | Peptide |
| 5 | h | 293 | PHE | Peptide |
| 5 | h | 320 | LEU | Peptide |
| 5 | h | 333 | GLY | Peptide |
| 5 | h | 361 | ASP | Peptide |
| 5 | h | 391 | GLY | Peptide |
| 5 | h | 61 | THR | Peptide |
| 5 | h | 84 | GLY | Peptide |
| 6 | i | 11 | ILE | Peptide |
| 6 | i | 8 | ALA | Peptide |
| 6 | i | 9 | GLY | Peptide |
| 6 | j | 11 | ILE | Peptide |
| 6 | j | 8 | ALA | Peptide |
| 6 | j | 9 | GLY | Peptide |
| 6 | k | 11 | ILE | Peptide |
| 6 | k | 8 | ALA | Peptide |
| 6 | k | 9 | GLY | Peptide |
| 7 | l | 28 | GLU | Peptide |
| 7 | l | 44 | VAL | Peptide |
| 7 | l | 46 | GLY | Peptide |
| 7 | l | 47 | VAL | Peptide |
| 7 | m | 152 | ALA | Peptide |
| 7 | m | 178 | PRO | Peptide |
| 7 | m | 28 | GLU | Peptide |
| 7 | m | 46 | GLY | Peptide |
| 7 | m | 47 | VAL | Peptide |
| 7 | m | 87 | TYR | Peptide |
| 7 | n | 152 | ALA | Peptide |
| 7 | n | 28 | GLU | Peptide |
| 7 | n | 47 | VAL | Peptide |
| 7 | n | 57 | ILE | Peptide |
| 7 | n | 86 | SER | Peptide |
| 10 | r | 340 | SER | Peptide |
| 11 | s | 2 | LEU | Peptide |
| 1 | u | 313 | ALA | Peptide |
| 1 | v | 136 | LYS | Peptide |
| 1 | v | 137 | ASP | Peptide |
| 1 | v | 18 | PRO | Peptide |
| 1 | v | 182 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | v | 20 | ILE | Peptide |
| 1 | v | 218 | GLY | Peptide |
| 1 | v | 256 | TYR | Peptide |
| 1 | v | 533 | ASP | Peptide |
| 2 | w | 105 | THR | Peptide |
| 2 | w | 134 | TYR | Peptide |
| 2 | w | 136 | ASN | Peptide |
| 2 | w | 156 | SER | Peptide |
| 2 | w | 167 | ILE | Peptide |
| 2 | w | 215 | LYS | Peptide |
| 2 | w | 227 | ASP | Peptide |
| 2 | w | 235 | LYS | Peptide |
| 2 | w | 298 | ALA | Peptide |
| 2 | w | 332 | SER | Peptide |
| 2 | w | 339 | ASP | Peptide |
| 2 | w | 342 | SER | Peptide |
| 2 | w | 343 | PRO | Peptide |
| 2 | w | 348 | ARG | Peptide |
| 2 | w | 353 | ASP | Peptide |
| 2 | w | 398 | SER | Peptide |
| 2 | w | 409 | ASP | Peptide |
| 2 | w | 436 | THR | Peptide |
| 2 | w | 456 | VAL | Peptide |
| 2 | w | 508 | TYR | Peptide |
| 2 | w | 554 | ASP | Peptide |
| 2 | w | 600 | PHE | Peptide |
| 2 | w | 623 | LEU | Peptide |
| 2 | w | 624 | GLN | Peptide |
| 2 | w | 625 | ASN | Peptide |
| 2 | w | 706 | SER | Peptide |
| 2 | w | 824 | GLN | Peptide |
| 2 | w | 850 | ASN | Peptide |
| 2 | w | 920 | LYS | Peptide |
| 2 | w | 925 | LEU | Peptide |
| 2 | w | 929 | TYR | Peptide |
| 2 | w | 940 | GLY | Peptide |
| 2 | w | 965 | LEU | Peptide |
| 2 | w | 967 | ASP | Peptide |
| 2 | w | 984 | SER | Peptide |
| 2 | w | 988 | LYS | Peptide |
| 2 | w | 989 | LEU | Peptide |
| 2 | w | 991 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | x | 102 | ASP | Peptide |
| 3 | x | 262 | ALA | Peptide |
| 3 | y | 177 | GLU | Peptide |
| 3 | y | 228 | ASN | Peptide |
| 3 | y | 32 | PRO | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5235 | 0 | 5086 | 352 | 0 |
| 1 | B | 5157 | 0 | 5011 | 344 | 0 |
| 1 | BH | 5235 | 0 | 5086 | 346 | 0 |
| 1 | BI | 5157 | 0 | 5011 | 350 | 0 |
| 1 | EA | 5235 | 0 | 5086 | 350 | 0 |
| 1 | EB | 5157 | 0 | 5011 | 355 | 0 |
| 1 | GD | 5235 | 0 | 5086 | 349 | 0 |
| 1 | GE | 5157 | 0 | 5011 | 345 | 0 |
| 1 | X | 5235 | 0 | 5086 | 345 | 0 |
| 1 | Y | 5157 | 0 | 5011 | 332 | 0 |
| 1 | u | 5235 | 0 | 5086 | 0 | 0 |
| 1 | v | 5157 | 0 | 5011 | 0 | 0 |
| 2 | BJ | 8199 | 0 | 7912 | 753 | 0 |
| 2 | C | 8199 | 0 | 7912 | 712 | 0 |
| 2 | EC | 8199 | 0 | 7912 | 744 | 0 |
| 2 | GF | 8199 | 0 | 7912 | 735 | 0 |
| 2 | Z | 8199 | 0 | 7912 | 641 | 0 |
| 2 | w | 8199 | 0 | 7912 | 0 | 0 |
| 3 | CA | 2631 | 0 | 2509 | 153 | 0 |
| 3 | CB | 2658 | 0 | 2534 | 131 | 0 |
| 3 | D | 2631 | 0 | 2509 | 160 | 0 |
| 3 | E | 2658 | 0 | 2534 | 140 | 0 |
| 3 | ED | 2631 | 0 | 2509 | 168 | 0 |
| 3 | EE | 2658 | 0 | 2534 | 142 | 0 |
| 3 | GG | 2631 | 0 | 2509 | 163 | 0 |
| 3 | GH | 2658 | 0 | 2534 | 136 | 0 |
| 3 | a | 2631 | 0 | 2509 | 0 | 0 |
| 3 | b | 2658 | 0 | 2534 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | x | 2631 | 0 | 2509 | 0 | 0 |
| 3 | y | 2658 | 0 | 2534 | 0 | 0 |
| 4 | AA | 2175 | 0 | 2157 | 102 | 0 |
| 4 | AB | 2175 | 0 | 2157 | 95 | 0 |
| 4 | CC | 2175 | 0 | 2157 | 113 | 0 |
| 4 | CD | 2175 | 0 | 2157 | 119 | 0 |
| 4 | CE | 2175 | 0 | 2157 | 117 | 0 |
| 4 | EF | 2175 | 0 | 2157 | 121 | 0 |
| 4 | EG | 2175 | 0 | 2157 | 120 | 0 |
| 4 | EH | 2175 | 0 | 2157 | 120 | 0 |
| 4 | F | 2175 | 0 | 2157 | 114 | 0 |
| 4 | G | 2175 | 0 | 2157 | 117 | 0 |
| 4 | GI | 2175 | 0 | 2157 | 120 | 0 |
| 4 | GJ | 2175 | 0 | 2157 | 115 | 0 |
| 4 | H | 2175 | 0 | 2157 | 113 | 0 |
| 4 | HA | 2175 | 0 | 2157 | 119 | 0 |
| 4 | c | 2175 | 0 | 2157 | 0 | 0 |
| 4 | d | 2175 | 0 | 2157 | 0 | 0 |
| 4 | e | 2175 | 0 | 2157 | 0 | 0 |
| 4 | z | 2175 | 0 | 2157 | 0 | 0 |
| 5 | AC | 4675 | 0 | 4446 | 445 | 0 |
| 5 | AD | 4675 | 0 | 4446 | 456 | 0 |
| 5 | AE | 4675 | 0 | 4446 | 468 | 0 |
| 5 | CF | 4675 | 0 | 4446 | 454 | 0 |
| 5 | CG | 4675 | 0 | 4446 | 473 | 0 |
| 5 | CH | 4675 | 0 | 4446 | 475 | 0 |
| 5 | EI | 4675 | 0 | 4446 | 462 | 0 |
| 5 | EJ | 4675 | 0 | 4446 | 470 | 0 |
| 5 | FA | 4675 | 0 | 4446 | 487 | 0 |
| 5 | HB | 4675 | 0 | 4446 | 467 | 0 |
| 5 | HC | 4675 | 0 | 4446 | 475 | 0 |
| 5 | HD | 4675 | 0 | 4446 | 475 | 0 |
| 5 | I | 4675 | 0 | 4446 | 457 | 0 |
| 5 | J | 4675 | 0 | 4446 | 460 | 0 |
| 5 | K | 4675 | 0 | 4446 | 483 | 0 |
| 5 | f | 4675 | 0 | 4446 | 0 | 0 |
| 5 | g | 4675 | 0 | 4446 | 0 | 0 |
| 5 | h | 4675 | 0 | 4446 | 0 | 0 |
| 6 | AF | 1665 | 0 | 1638 | 119 | 0 |
| 6 | AG | 1665 | 0 | 1638 | 101 | 0 |
| 6 | AH | 1665 | 0 | 1638 | 106 | 0 |
| 6 | CI | 1665 | 0 | 1638 | 110 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 6 | CJ | 1665 | 0 | 1638 | 101 | 0 |
| 6 | DA | 1665 | 0 | 1638 | 99 | 0 |
| 6 | FB | 1665 | 0 | 1638 | 113 | 0 |
| 6 | FC | 1665 | 0 | 1638 | 107 | 0 |
| 6 | FD | 1665 | 0 | 1638 | 107 | 0 |
| 6 | HE | 1665 | 0 | 1638 | 109 | 0 |
| 6 | HF | 1665 | 0 | 1638 | 102 | 0 |
| 6 | HG | 1665 | 0 | 1638 | 108 | 0 |
| 6 | L | 1665 | 0 | 1638 | 104 | 0 |
| 6 | M | 1665 | 0 | 1638 | 106 | 0 |
| 6 | N | 1665 | 0 | 1638 | 107 | 0 |
| 6 | i | 1665 | 0 | 1638 | 0 | 0 |
| 6 | j | 1665 | 0 | 1638 | 0 | 0 |
| 6 | k | 1665 | 0 | 1638 | 0 | 0 |
| 7 | AI | 3945 | 0 | 3828 | 399 | 0 |
| 7 | AJ | 3945 | 0 | 3828 | 389 | 0 |
| 7 | BA | 3945 | 0 | 3828 | 419 | 0 |
| 7 | DB | 3945 | 0 | 3828 | 407 | 0 |
| 7 | DC | 3945 | 0 | 3828 | 398 | 0 |
| 7 | DD | 3945 | 0 | 3828 | 421 | 0 |
| 7 | FE | 3945 | 0 | 3828 | 412 | 0 |
| 7 | FF | 3945 | 0 | 3828 | 396 | 0 |
| 7 | FG | 3945 | 0 | 3828 | 427 | 0 |
| 7 | HH | 3945 | 0 | 3828 | 401 | 0 |
| 7 | HI | 3945 | 0 | 3828 | 401 | 0 |
| 7 | HJ | 3945 | 0 | 3828 | 425 | 0 |
| 7 | O | 3945 | 0 | 3828 | 410 | 0 |
| 7 | P | 3945 | 0 | 3828 | 403 | 0 |
| 7 | Q | 3945 | 0 | 3828 | 424 | 0 |
| 7 | l | 3945 | 0 | 3828 | 0 | 0 |
| 7 | m | 3945 | 0 | 3828 | 0 | 0 |
| 7 | n | 3945 | 0 | 3828 | 0 | 0 |
| 8 | BB | 1296 | 0 | 1243 | 80 | 0 |
| 8 | BC | 1296 | 0 | 1243 | 76 | 0 |
| 8 | DE | 1296 | 0 | 1243 | 89 | 0 |
| 8 | DF | 1296 | 0 | 1243 | 89 | 0 |
| 8 | FH | 1296 | 0 | 1243 | 92 | 0 |
| 8 | FI | 1296 | 0 | 1243 | 90 | 0 |
| 8 | IA | 1296 | 0 | 1243 | 88 | 0 |
| 8 | IB | 1296 | 0 | 1243 | 94 | 0 |
| 8 | R | 1296 | 0 | 1243 | 77 | 0 |
| 8 | S | 1296 | 0 | 1243 | 78 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 8 | o | 1296 | 0 | 1243 | 0 | 0 |
| 8 | p | 1296 | 0 | 1243 | 0 | 0 |
| 9 | BD | 1011 | 0 | 1009 | 38 | 0 |
| 9 | DG | 1011 | 0 | 1009 | 51 | 0 |
| 9 | FJ | 1011 | 0 | 1009 | 50 | 0 |
| 9 | IC | 1011 | 0 | 1009 | 51 | 0 |
| 9 | T | 1011 | 0 | 1009 | 47 | 0 |
| 9 | q | 1011 | 0 | 1009 | 0 | 0 |
| 10 | BE | 1317 | 0 | 1296 | 72 | 0 |
| 10 | DH | 1317 | 0 | 1296 | 79 | 0 |
| 10 | GA | 1317 | 0 | 1296 | 78 | 0 |
| 10 | ID | 1317 | 0 | 1296 | 86 | 0 |
| 10 | U | 1317 | 0 | 1296 | 83 | 0 |
| 10 | r | 1317 | 0 | 1296 | 0 | 0 |
| 11 | BF | 1599 | 0 | 1544 | 89 | 0 |
| 11 | DI | 1599 | 0 | 1544 | 114 | 0 |
| 11 | GB | 1599 | 0 | 1544 | 108 | 0 |
| 11 | IE | 1599 | 0 | 1544 | 108 | 0 |
| 11 | V | 1599 | 0 | 1544 | 112 | 0 |
| 11 | s | 1599 | 0 | 1544 | 0 | 0 |
| 12 | BG | 1524 | 0 | 1439 | 117 | 0 |
| 12 | DJ | 1524 | 0 | 1439 | 135 | 0 |
| 12 | GC | 1524 | 0 | 1439 | 136 | 0 |
| 12 | IF | 1524 | 0 | 1439 | 140 | 0 |
| 12 | W | 1524 | 0 | 1439 | 109 | 0 |
| 12 | t | 1524 | 0 | 1439 | 0 | 0 |
| 13 | YA | 25692 | 0 | 21556 | 1614 | 0 |
| 13 | YB | 25692 | 0 | 21769 | 1791 | 0 |
| 13 | YC | 25692 | 0 | 21586 | 1892 | 0 |
| 14 | YD | 17472 | 0 | 15252 | 1037 | 0 |
| 14 | YE | 17472 | 0 | 15217 | 1072 | 0 |
| 14 | YF | 17472 | 0 | 15224 | 1053 | 0 |
| 15 | ZA | 4254 | 0 | 4245 | 108 | 0 |
| 16 | AI | 1 | 0 | 0 | 0 | 0 |
| 16 | DB | 1 | 0 | 0 | 0 | 0 |
| 16 | FE | 1 | 0 | 0 | 0 | 0 |
| 16 | HH | 1 | 0 | 0 | 0 | 0 |
| 16 | O | 1 | 0 | 0 | 0 | 0 |
| 16 | l | 1 | 0 | 0 | 0 | 0 |
| 17 | ZA | 6 | 0 | 0 | 0 | 0 |
| All | All | 549576 | 0 | 517047 | 29063 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 32.

All (29063) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:24:ASN:HD22 | 7:Q:41:PRO:HA | 1.18 | 1.06 |
| 2:BJ:935:LYS:HD2 | 2:BJ:954:GLU:HG2 | 1.39 | 1.04 |
| 7:FE:24:ASN:HD22 | 7:FG:41:PRO:HA | 1.17 | 1.04 |
| 2:EC:935:LYS:HD2 | 2:EC:954:GLU:HG2 | 1.39 | 1.04 |
| 7:AI:24:ASN:HD22 | 7:BA:41:PRO:HA | 1.17 | 1.03 |
| 2:GF:935:LYS:HD2 | 2:GF:954:GLU:HG2 | 1.39 | 1.03 |
| 7:HH:24:ASN:HD22 | 7:HJ:41:PRO:HA | 1.17 | 1.03 |
| 1:A:338:ARG:HG2 | 1:B:336:GLN:HE22 | 1.23 | 1.03 |
| 2:Z:935:LYS:HD2 | 2:Z:954:GLU:HG2 | 1.39 | 1.02 |
| 8:R:77:GLU:HA | 8:IA:16:ALA:HB2 | 1.41 | 1.02 |
| 2:C:935:LYS:HD2 | 2:C:954:GLU:HG2 | 1.39 | 1.01 |
| 7:DB:24:ASN:HD22 | 7:DD:41:PRO:HA | 1.22 | 1.01 |
| 8:DE:16:ALA:HB2 | 8:FH:77:GLU:HA | 1.43 | 1.01 |
| 1:X:338:ARG:HG2 | 1:Y:336:GLN:HE22 | 1.22 | 1.01 |
| 13:YB:61[D]:ILE:HG21 | 13:YC:59[D]:GLN:HA | 1.40 | 1.01 |
| 1:GD:338:ARG:HG2 | 1:GE:336:GLN:HE22 | 1.25 | 1.00 |
| 15:ZA:26[D]:GLN:HE22 | 15:ZA:29[D]:VAL:H | 1.08 | 1.00 |
| 2:EC:646:ARG:HD2 | 2:EC:673:GLN:HE22 | 1.28 | 0.99 |
| 2:C:646:ARG:HD2 | 2:C:673:GLN:HE22 | 1.28 | 0.99 |
| 1:EA:338:ARG:HG2 | 1:EB:336:GLN:HE22 | 1.23 | 0.99 |
| 1:BH:338:ARG:HG2 | 1:BI:336:GLN:HE22 | 1.24 | 0.99 |
| 13:YB:61[A]:ILE:HG21 | 13:YC:59[A]:GLN:HA | 1.40 | 0.99 |
| 2:Z:646:ARG:HD2 | 2:Z:673:GLN:HE22 | 1.28 | 0.98 |
| 5:HB:315:GLY:HA3 | 5:HD:316:ILE:HG23 | 1.44 | 0.98 |
| 8:BB:16:ALA:HB2 | 8:DE:77:GLU:HA | 1.44 | 0.98 |
| 6:M:10:VAL:HA | 6:N:13:ARG:HD2 | 1.46 | 0.97 |
| 2:EC:302:ALA:O | 2:EC:327:ARG:NH1 | 1.96 | 0.97 |
| 2:GF:302:ALA:O | 2:GF:327:ARG:NH1 | 1.96 | 0.97 |
| 2:BJ:302:ALA:O | 2:BJ:327:ARG:NH1 | 1.96 | 0.97 |
| 15:ZA:26[C]:GLN:HE22 | 15:ZA:29[C]:VAL:H | 1.08 | 0.97 |
| 2:GF:646:ARG:HD2 | 2:GF:673:GLN:HE22 | 1.28 | 0.97 |
| 2:Z:302:ALA:O | 2:Z:327:ARG:NH1 | 1.96 | 0.97 |
| 2:C:302:ALA:O | 2:C:327:ARG:NH1 | 1.96 | 0.97 |
| 15:ZA:26[E]:GLN:HE22 | 15:ZA:29[E]:VAL:H | 1.08 | 0.96 |
| 8:FH:16:ALA:HB2 | 8:IA:77:GLU:HA | 1.43 | 0.96 |
| 2:Z:351:GLU:HB2 | 2:Z:353:ASP:HB2 | 1.47 | 0.96 |
| 5:I:323:THR:N | 5:I:358:VAL:O | 1.98 | 0.96 |
| 2:BJ:351:GLU:HB2 | 2:BJ:353:ASP:HB2 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:646:ARG:HD2 | 2:BJ:673:GLN:HE22 | 1.28 | 0.96 |
| 6:CJ:10:VAL:HA | 6:DA:13:ARG:HD2 | 1.47 | 0.96 |
| 2:C:351:GLU:HB2 | 2:C:353:ASP:HB2 | 1.47 | 0.96 |
| 15:ZA:26[F]:GLN:HE22 | 15:ZA:29[F]:VAL:H | 1.08 | 0.96 |
| 13:YA:59[A]:GLN:HA | 13:YC:61[A]:ILE:HG21 | 1.46 | 0.95 |
| 5:EI:323:THR:N | 5:EI:358:VAL:O | 1.98 | 0.95 |
| 2:GF:351:GLU:HB2 | 2:GF:353:ASP:HB2 | 1.47 | 0.95 |
| 13:YA:59[D]:GLN:HA | 13:YC:61[D]:ILE:HG21 | 1.46 | 0.95 |
| 6:FC:10:VAL:HA | 6:FD:13:ARG:HD2 | 1.47 | 0.95 |
| 6:AG:10:VAL:HA | 6:AH:13:ARG:HD2 | 1.49 | 0.95 |
| 5:CF:323:THR:N | 5:CF:358:VAL:O | 1.98 | 0.94 |
| 2:EC:351:GLU:HB2 | 2:EC:353:ASP:HB2 | 1.47 | 0.94 |
| 5:AC:323:THR:N | 5:AC:358:VAL:O | 1.98 | 0.94 |
| 5:EJ:285:LEU:HD11 | 5:EJ:375:PHE:HB2 | 1.49 | 0.94 |
| 5:CG:285:LEU:HD11 | 5:CG:375:PHE:HB2 | 1.49 | 0.94 |
| 5:HB:34:TYR:OH | 5:HB:40:GLY:O | 1.86 | 0.94 |
| 5:HB:304:ILE:HD12 | 5:HB:385:TRP:HA | 1.50 | 0.94 |
| 5:EI:304:ILE:HD12 | 5:EI:385:TRP:HA | 1.50 | 0.93 |
| 5:AC:304:ILE:HD12 | 5:AC:385:TRP:HA | 1.50 | 0.93 |
| 5:CH:326:MET:HG3 | 5:CH:327:PRO:HD3 | 1.51 | 0.93 |
| 5:HB:323:THR:N | 5:HB:358:VAL:O | 1.98 | 0.93 |
| 13:YA:321[C]:LYS:HD3 | 13:YB:452[C]:GLY:HA2 | 1.51 | 0.93 |
| 5:AE:326:MET:HG3 | 5:AE:327:PRO:HD3 | 1.51 | 0.93 |
| 5:CF:304:ILE:HD12 | 5:CF:385:TRP:HA | 1.50 | 0.93 |
| 2:EC:75:LEU:N | 2:EC:102:THR:O | 2.02 | 0.93 |
| 5:HC:285:LEU:HD11 | 5:HC:375:PHE:HB2 | 1.49 | 0.93 |
| 5:K:326:MET:HG3 | 5:K:327:PRO:HD3 | 1.51 | 0.93 |
| 2:BJ:75:LEU:N | 2:BJ:102:THR:O | 2.02 | 0.93 |
| 5:I:304:ILE:HD12 | 5:I:385:TRP:HA | 1.50 | 0.93 |
| 13:YA:321[F]:LYS:HD3 | 13:YB:452[F]:GLY:HA2 | 1.51 | 0.93 |
| 5:AD:285:LEU:HD11 | 5:AD:375:PHE:HB2 | 1.49 | 0.92 |
| 5:EI:34:TYR:OH | 5:EI:40:GLY:O | 1.86 | 0.92 |
| 5:J:285:LEU:HD11 | 5:J:375:PHE:HB2 | 1.49 | 0.92 |
| 15:ZA:26[A]:GLN:HE22 | 15:ZA:29[A]:VAL:H | 1.08 | 0.92 |
| 2:GF:75:LEU:N | 2:GF:102:THR:O | 2.02 | 0.92 |
| 7:DB:98:THR:HG1 | 7:DD:100:TYR:HH | 0.93 | 0.92 |
| 13:YA:321[B]:LYS:HD3 | 13:YB:452[B]:GLY:HA2 | 1.51 | 0.92 |
| 15:ZA:26[B]:GLN:HE22 | 15:ZA:29[B]:VAL:H | 1.08 | 0.92 |
| 5:I:34:TYR:OH | 5:I:40:GLY:O | 1.86 | 0.92 |
| 13:YB:61[C]:ILE:HG21 | 13:YC:59[C]:GLN:HA | 1.52 | 0.92 |
| 5:CF:34:TYR:OH | 5:CF:40:GLY:O | 1.86 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HF:10:VAL:HA | 6:HG:13:ARG:HD2 | 1.52 | 0.92 |
| 13:YA:321[E]:LYS:HD3 | 13:YB:452[E]:GLY:HA2 | 1.51 | 0.92 |
| 5:HB:359:GLU:HB3 | 5:HB:370:HIS:HB3 | 1.52 | 0.92 |
| 2:C:75:LEU:N | 2:C:102:THR:O | 2.02 | 0.91 |
| 5:EI:359:GLU:HB3 | 5:EI:370:HIS:HB3 | 1.52 | 0.91 |
| 5:FA:326:MET:HG3 | 5:FA:327:PRO:HD3 | 1.51 | 0.91 |
| 5:CF:359:GLU:HB3 | 5:CF:370:HIS:HB3 | 1.52 | 0.91 |
| 7:DB:335:ASN:H | 7:DC:329:ASN:HD21 | 1.18 | 0.91 |
| 2:C:120:ASN:HB2 | 2:C:155:PRO:HB3 | 1.52 | 0.91 |
| 5:HD:326:MET:HG3 | 5:HD:327:PRO:HD3 | 1.51 | 0.91 |
| 5:AC:34:TYR:OH | 5:AC:40:GLY:O | 1.86 | 0.91 |
| 2:BJ:872:SER:H | 2:BJ:894:THR:HG21 | 1.35 | 0.91 |
| 8:DF:16:ALA:HB2 | 8:FI:77:GLU:HA | 1.51 | 0.91 |
| 5:I:359:GLU:HB3 | 5:I:370:HIS:HB3 | 1.52 | 0.91 |
| 2:Z:75:LEU:N | 2:Z:102:THR:O | 2.02 | 0.91 |
| 7:O:335:ASN:H | 7:P:329:ASN:HD21 | 1.18 | 0.91 |
| 13:YA:61[A]:ILE:HG21 | 13:YB:59[A]:GLN:HA | 1.52 | 0.91 |
| 5:AC:359:GLU:HB3 | 5:AC:370:HIS:HB3 | 1.52 | 0.91 |
| 13:YB:61[E]:ILE:HG21 | 13:YC:59[E]:GLN:HA | 1.51 | 0.91 |
| 5:I:315:GLY:HA3 | 5:K:316:ILE:HG23 | 1.53 | 0.91 |
| 13:YB:47[C]:ILE:HG23 | 14:YE:123[C]:PRO:HG3 | 1.53 | 0.91 |
| 4:GI:248:GLU:HG3 | 4:GI:249:ILE:HG13 | 1.54 | 0.91 |
| 7:Q:352:ASP:HB3 | 7:HI:53:THR:HG21 | 1.53 | 0.91 |
| 5:EI:315:GLY:HA3 | 5:FA:316:ILE:HG23 | 1.54 | 0.90 |
| 7:AI:335:ASN:H | 7:AJ:329:ASN:HD21 | 1.19 | 0.90 |
| 2:GF:333:ASN:HB2 | 4:GI:18:ALA:HA | 1.53 | 0.90 |
| 7:HH:29:ILE:HG22 | 7:HH:30:THR:H | 1.37 | 0.90 |
| 2:EC:872:SER:H | 2:EC:894:THR:HG21 | 1.35 | 0.90 |
| 4:EG:248:GLU:HG3 | 4:EG:249:ILE:HG13 | 1.53 | 0.90 |
| 4:H:248:GLU:HG3 | 4:H:249:ILE:HG13 | 1.53 | 0.90 |
| 5:HC:323:THR:N | 5:HC:358:VAL:O | 2.04 | 0.90 |
| 13:YB:47[B]:ILE:HG23 | 14:YE:123[B]:PRO:HG3 | 1.53 | 0.90 |
| 5:EI:394:LEU:HD21 | 5:EI:399:ILE:HD11 | 1.53 | 0.90 |
| 7:HI:4:ASN:OD1 | 7:HI:15:TYR:OH | 1.90 | 0.90 |
| 13:YA:321[D]:LYS:HD3 | 13:YB:452[D]:GLY:HA2 | 1.51 | 0.90 |
| 2:Z:120:ASN:HB2 | 2:Z:155:PRO:HB3 | 1.52 | 0.90 |
| 2:Z:872:SER:H | 2:Z:894:THR:HG21 | 1.35 | 0.90 |
| 4:EF:248:GLU:HG3 | 4:EF:249:ILE:HG13 | 1.53 | 0.90 |
| 5:HB:393:LEU:HD11 | 5:HD:391:GLY:HA2 | 1.53 | 0.90 |
| 13:YA:321[A]:LYS:HD3 | 13:YB:452[A]:GLY:HA2 | 1.51 | 0.90 |
| 4:CD:248:GLU:HG3 | 4:CD:249:ILE:HG13 | 1.53 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:248:GLU:HG3 | 4:F:249:ILE:HG13 | 1.53 | 0.90 |
| 8:FI:16:ALA:HB2 | 8:IB:77:GLU:HA | 1.51 | 0.90 |
| 4:AA:248:GLU:HG3 | 4:AA:249:ILE:HG13 | 1.53 | 0.90 |
| 4:CC:248:GLU:HG3 | 4:CC:249:ILE:HG13 | 1.53 | 0.90 |
| 2:GF:872:SER:H | 2:GF:894:THR:HG21 | 1.35 | 0.90 |
| 1:BI:582:ASN:HD21 | 1:BI:586:ARG:HH21 | 1.18 | 0.89 |
| 2:BJ:120:ASN:HB2 | 2:BJ:155:PRO:HB3 | 1.52 | 0.89 |
| 7:DB:29:ILE:HG22 | 7:DB:30:THR:H | 1.37 | 0.89 |
| 5:J:323:THR:N | 5:J:358:VAL:O | 2.04 | 0.89 |
| 4:HA:248:GLU:HG3 | 4:HA:249:ILE:HG13 | 1.54 | 0.89 |
| 7:HH:335:ASN:H | 7:HI:329:ASN:HD21 | 1.19 | 0.89 |
| 13:YB:47[F]:ILE:HG23 | 14:YE:123[F]:PRO:HG3 | 1.54 | 0.89 |
| 13:YA:61[D]:ILE:HG21 | 13:YB:59[D]:GLN:HA | 1.52 | 0.89 |
| 5:AD:323:THR:N | 5:AD:358:VAL:O | 2.04 | 0.89 |
| 4:AB:248:GLU:HG3 | 4:AB:249:ILE:HG13 | 1.53 | 0.89 |
| 2:C:872:SER:H | 2:C:894:THR:HG21 | 1.35 | 0.89 |
| 1:GD:252:LEU:O | 1:GE:335:THR:OG1 | 1.91 | 0.89 |
| 13:YB:7[D]:ASN:HD21 | 13:YC:9[D]:ASN:HA | 1.37 | 0.89 |
| 5:CF:394:LEU:HD21 | 5:CF:399:ILE:HD11 | 1.53 | 0.89 |
| 8:BC:16:ALA:HB2 | 8:DF:77:GLU:HA | 1.53 | 0.89 |
| 7:FE:441:GLN:HE21 | 7:FG:509:GLY:HA3 | 1.37 | 0.89 |
| 5:I:394:LEU:HD21 | 5:I:399:ILE:HD11 | 1.53 | 0.89 |
| 13:YB:7[F]:ASN:HD21 | 13:YC:9[F]:ASN:HA | 1.38 | 0.89 |
| 3:ED:43:ARG:NH1 | 3:ED:45:GLU:O | 2.06 | 0.89 |
| 13:YB:7[C]:ASN:HD21 | 13:YC:9[C]:ASN:HA | 1.38 | 0.89 |
| 7:FE:335:ASN:H | 7:FF:329:ASN:HD21 | 1.20 | 0.89 |
| 7:FF:4:ASN:OD1 | 7:FF:15:TYR:OH | 1.90 | 0.89 |
| 13:YB:47[D]:ILE:HG23 | 14:YE:123[D]:PRO:HG3 | 1.52 | 0.89 |
| 5:AC:394:LEU:HD21 | 5:AC:399:ILE:HD11 | 1.53 | 0.89 |
| 1:EA:252:LEU:O | 1:EB:335:THR:OG1 | 1.90 | 0.89 |
| 13:YB:7[E]:ASN:HD21 | 13:YC:9[E]:ASN:HA | 1.37 | 0.89 |
| 3:GG:43:ARG:NH1 | 3:GG:45:GLU:O | 2.06 | 0.88 |
| 7:P:4:ASN:OD1 | 7:P:15:TYR:OH | 1.90 | 0.88 |
| 7:AJ:4:ASN:OD1 | 7:AJ:15:TYR:OH | 1.90 | 0.88 |
| 1:BH:67:ILE:HD11 | 1:BI:67:ILE:HD13 | 1.54 | 0.88 |
| 5:CG:323:THR:N | 5:CG:358:VAL:O | 2.04 | 0.88 |
| 5:EJ:323:THR:N | 5:EJ:358:VAL:O | 2.05 | 0.88 |
| 4:GJ:248:GLU:HG3 | 4:GJ:249:ILE:HG13 | 1.53 | 0.88 |
| 5:HB:394:LEU:HD21 | 5:HB:399:ILE:HD11 | 1.53 | 0.88 |
| 8:S:77:GLU:HA | 8:IB:16:ALA:HB2 | 1.54 | 0.88 |
| 4:CE:248:GLU:HG3 | 4:CE:249:ILE:HG13 | 1.53 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:120:ASN:HB2 | 2:EC:155:PRO:HB3 | 1.52 | 0.88 |
| 7:FE:29:ILE:HG22 | 7:FE:30:THR:H | 1.37 | 0.88 |
| 13:YB:47[E]:ILE:HG23 | 14:YE:123[E]:PRO:HG3 | 1.53 | 0.88 |
| 4:G:248:GLU:HG3 | 4:G:249:ILE:HG13 | 1.53 | 0.88 |
| 5:HC:191:ILE:O | 5:HD:164:ARG:NH2 | 2.06 | 0.88 |
| 7:HH:441:GLN:HE21 | 7:HJ:509:GLY:HA3 | 1.39 | 0.88 |
| 13:YB:7[B]:ASN:HD21 | 13:YC:9[B]:ASN:HA | 1.37 | 0.88 |
| 1:X:252:LEU:O | 1:Y:335:THR:OG1 | 1.90 | 0.88 |
| 13:YB:47[A]:ILE:HG23 | 14:YE:123[A]:PRO:HG3 | 1.53 | 0.88 |
| 7:AJ:167:GLN:O | 7:AJ:171:LYS:N | 2.07 | 0.88 |
| 7:DC:167:GLN:O | 7:DC:171:LYS:N | 2.07 | 0.88 |
| 7:O:29:ILE:HG22 | 7:O:30:THR:H | 1.37 | 0.88 |
| 13:YC:423[C]:GLU:OE1 | 13:YC:429[C]:ARG:NH2 | 2.07 | 0.88 |
| 1:B:582:ASN:HD21 | 1:B:586:ARG:HH21 | 1.18 | 0.88 |
| 1:GE:582:ASN:HD21 | 1:GE:586:ARG:HH21 | 1.18 | 0.88 |
| 13:YB:423[F]:GLU:OE1 | 13:YB:429[F]:ARG:NH2 | 2.07 | 0.88 |
| 7:DC:4:ASN:OD1 | 7:DC:15:TYR:OH | 1.90 | 0.88 |
| 1:EB:582:ASN:HD21 | 1:EB:586:ARG:HH21 | 1.18 | 0.88 |
| 4:EH:248:GLU:HG3 | 4:EH:249:ILE:HG13 | 1.53 | 0.88 |
| 13:YA:423[B]:GLU:OE1 | 13:YA:429[B]:ARG:NH2 | 2.07 | 0.88 |
| 13:YB:423[E]:GLU:OE1 | 13:YB:429[E]:ARG:NH2 | 2.07 | 0.88 |
| 7:AI:29:ILE:HG22 | 7:AI:30:THR:H | 1.37 | 0.88 |
| 1:A:252:LEU:O | 1:B:335:THR:OG1 | 1.91 | 0.88 |
| 7:DD:29:ILE:HG22 | 7:DD:30:THR:H | 1.39 | 0.88 |
| 7:AI:441:GLN:HE21 | 7:BA:509:GLY:HA3 | 1.39 | 0.87 |
| 5:CF:315:GLY:HA3 | 5:CH:316:ILE:HG23 | 1.55 | 0.87 |
| 13:YA:423[C]:GLU:OE1 | 13:YA:429[C]:ARG:NH2 | 2.07 | 0.87 |
| 13:YA:9[D]:ASN:HA | 13:YC:7[D]:ASN:HD21 | 1.39 | 0.87 |
| 7:FF:167:GLN:O | 7:FF:171:LYS:N | 2.07 | 0.87 |
| 2:GF:120:ASN:HB2 | 2:GF:155:PRO:HB3 | 1.52 | 0.87 |
| 13:YC:423[B]:GLU:OE1 | 13:YC:429[B]:ARG:NH2 | 2.07 | 0.87 |
| 13:YA:423[F]:GLU:OE1 | 13:YA:429[F]:ARG:NH2 | 2.07 | 0.87 |
| 7:HJ:29:ILE:HG22 | 7:HJ:30:THR:H | 1.39 | 0.87 |
| 3:CA:43:ARG:NH1 | 3:CA:45:GLU:O | 2.06 | 0.87 |
| 7:HI:167:GLN:O | 7:HI:171:LYS:N | 2.07 | 0.87 |
| 7:P:167:GLN:O | 7:P:171:LYS:N | 2.07 | 0.87 |
| 13:YC:423[D]:GLU:OE1 | 13:YC:429[D]:ARG:NH2 | 2.08 | 0.87 |
| 13:YC:423[E]:GLU:OE1 | 13:YC:429[E]:ARG:NH2 | 2.07 | 0.87 |
| 7:FG:29:ILE:HG22 | 7:FG:30:THR:H | 1.39 | 0.87 |
| 13:YB:423[C]:GLU:OE1 | 13:YB:429[C]:ARG:NH2 | 2.07 | 0.87 |
| 13:YC:423[F]:GLU:OE1 | 13:YC:429[F]:ARG:NH2 | 2.07 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:125[A]:PHE:HE2 | 14:YE:134[A]:GLU:HG3 | 1.40 | 0.87 |
| 13:YA:423[A]:GLU:OE1 | 13:YA:429[A]:ARG:NH2 | 2.08 | 0.87 |
| 13:YA:423[E]:GLU:OE1 | 13:YA:429[E]:ARG:NH2 | 2.07 | 0.87 |
| 13:YB:423[A]:GLU:OE1 | 13:YB:429[A]:ARG:NH2 | 2.08 | 0.87 |
| 5:AC:215:PRO:HG3 | 5:AC:226:ASP:HB2 | 1.57 | 0.87 |
| 13:YB:423[B]:GLU:OE1 | 13:YB:429[B]:ARG:NH2 | 2.07 | 0.87 |
| 14:YD:125[C]:PHE:HE2 | 14:YD:134[C]:GLU:HG3 | 1.40 | 0.87 |
| 13:YA:423[D]:GLU:OE1 | 13:YA:429[D]:ARG:NH2 | 2.08 | 0.87 |
| 14:YF:125[E]:PHE:HE2 | 14:YF:134[E]:GLU:HG3 | 1.40 | 0.87 |
| 3:D:43:ARG:NH1 | 3:D:45:GLU:O | 2.06 | 0.86 |
| 5:K:193:VAL:HG13 | 5:K:199:GLU:HB3 | 1.57 | 0.86 |
| 13:YC:423[A]:GLU:OE1 | 13:YC:429[A]:ARG:NH2 | 2.08 | 0.86 |
| 5:HB:49:TRP:O | 5:HD:90:ASN:ND2 | 2.08 | 0.86 |
| 1:Y:98:TYR:HB2 | 1:Y:332:LYS:HG3 | 1.57 | 0.86 |
| 13:YA:59[C]:GLN:HA | 13:YC:61[C]:ILE:HG21 | 1.56 | 0.86 |
| 13:YA:9[F]:ASN:HA | 13:YC:7[F]:ASN:HD21 | 1.40 | 0.86 |
| 2:Z:300:LEU:HD22 | 2:Z:329:ILE:HD13 | 1.58 | 0.86 |
| 13:YB:423[D]:GLU:OE1 | 13:YB:429[D]:ARG:NH2 | 2.08 | 0.86 |
| 1:B:98:TYR:HB2 | 1:B:332:LYS:HG3 | 1.57 | 0.86 |
| 1:BI:98:TYR:HB2 | 1:BI:332:LYS:HG3 | 1.57 | 0.86 |
| 5:FA:193:VAL:HG13 | 5:FA:199:GLU:HB3 | 1.57 | 0.86 |
| 7:O:399:PHE:HE1 | 7:P:401:ARG:HB3 | 1.40 | 0.86 |
| 7:O:441:GLN:HE21 | 7:Q:509:GLY:HA3 | 1.40 | 0.86 |
| 5:J:285:LEU:HD21 | 5:J:375:PHE:H | 1.41 | 0.86 |
| 7:O:98:THR:HG1 | 7:Q:100:TYR:HH | 0.86 | 0.86 |
| 7:Q:29:ILE:HG22 | 7:Q:30:THR:H | 1.39 | 0.86 |
| 1:EA:67:ILE:HD11 | 1:EB:67:ILE:HD13 | 1.57 | 0.86 |
| 1:X:338:ARG:HG2 | 1:Y:336:GLN:NE2 | 1.91 | 0.86 |
| 13:YA:9[B]:ASN:HA | 13:YC:7[B]:ASN:HD21 | 1.39 | 0.86 |
| 1:BH:252:LEU:O | 1:BI:335:THR:OG1 | 1.93 | 0.86 |
| 1:GD:67:ILE:HD11 | 1:GE:67:ILE:HD13 | 1.57 | 0.86 |
| 13:YA:9[A]:ASN:HA | 13:YC:7[A]:ASN:HD21 | 1.39 | 0.86 |
| 5:AE:193:VAL:HG13 | 5:AE:199:GLU:HB3 | 1.57 | 0.86 |
| 7:DB:441:GLN:HE21 | 7:DD:509:GLY:HA3 | 1.39 | 0.86 |
| 5:AE:111:ALA:HB2 | 5:AE:117:ILE:HG23 | 1.58 | 0.85 |
| 7:DC:399:PHE:CE1 | 7:DD:401:ARG:HB3 | 2.11 | 0.85 |
| 7:FF:53:THR:HG21 | 7:HJ:352:ASP:HB3 | 1.58 | 0.85 |
| 14:YD:125[A]:PHE:HE2 | 14:YD:134[A]:GLU:HG3 | 1.40 | 0.85 |
| 5:AC:315:GLY:HA3 | 5:AE:316:ILE:HG23 | 1.54 | 0.85 |
| 2:GF:255:TYR:HB2 | 2:GF:297:TYR:HB2 | 1.59 | 0.85 |
| 7:BA:29:ILE:HG22 | 7:BA:30:THR:H | 1.39 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:111:ALA:HB2 | 5:CH:117:ILE:HG23 | 1.58 | 0.85 |
| 5:CH:323:THR:N | 5:CH:358:VAL:O | 2.09 | 0.85 |
| 5:FA:111:ALA:HB2 | 5:FA:117:ILE:HG23 | 1.58 | 0.85 |
| 5:HC:285:LEU:HD21 | 5:HC:375:PHE:H | 1.41 | 0.85 |
| 5:HD:111:ALA:HB2 | 5:HD:117:ILE:HG23 | 1.58 | 0.85 |
| 7:HI:399:PHE:CE1 | 7:HJ:401:ARG:HB3 | 2.11 | 0.85 |
| 14:YE:125[E]:PHE:HE2 | 14:YE:134[E]:GLU:HG3 | 1.40 | 0.85 |
| 2:EC:255:TYR:HB2 | 2:EC:297:TYR:HB2 | 1.59 | 0.85 |
| 1:Y:194:ARG:NH2 | 1:Y:228:GLU:OE2 | 2.10 | 0.85 |
| 1:Y:582:ASN:HD21 | 1:Y:586:ARG:HH21 | 1.18 | 0.85 |
| 1:X:63:ASN:HD22 | 1:Y:60:LEU:HB3 | 1.39 | 0.85 |
| 13:YB:7[A]:ASN:HD21 | 13:YC:9[A]:ASN:HA | 1.37 | 0.85 |
| 14:YF:125[C]:PHE:HE2 | 14:YF:134[C]:GLU:HG3 | 1.40 | 0.85 |
| 5:CH:193:VAL:HG13 | 5:CH:199:GLU:HB3 | 1.57 | 0.85 |
| 5:K:323:THR:N | 5:K:358:VAL:O | 2.09 | 0.85 |
| 13:YA:59[E]:GLN:HA | 13:YC:61[E]:ILE:HG21 | 1.58 | 0.85 |
| 13:YA:9[C]:ASN:HA | 13:YC:7[C]:ASN:HD21 | 1.40 | 0.85 |
| 1:A:67:ILE:HD11 | 1:B:67:ILE:HD13 | 1.57 | 0.85 |
| 2:C:300:LEU:HD22 | 2:C:329:ILE:HD13 | 1.58 | 0.85 |
| 2:EC:580:LYS:HG2 | 2:EC:581:TYR:H | 1.42 | 0.85 |
| 1:GE:98:TYR:HB2 | 1:GE:332:LYS:HG3 | 1.57 | 0.85 |
| 5:HD:323:THR:N | 5:HD:358:VAL:O | 2.09 | 0.85 |
| 7:AI:98:THR:HG1 | 7:BA:100:TYR:HH | 0.88 | 0.85 |
| 7:AJ:399:PHE:CE1 | 7:BA:401:ARG:HB3 | 2.11 | 0.85 |
| 5:CG:285:LEU:HD21 | 5:CG:375:PHE:H | 1.41 | 0.85 |
| 5:EJ:285:LEU:HD21 | 5:EJ:375:PHE:H | 1.41 | 0.85 |
| 5:AC:103:ASN:N | 5:AC:127:ASN:O | 2.10 | 0.85 |
| 3:CA:115:ASN:HA | 3:CA:121:ALA:HA | 1.59 | 0.85 |
| 2:EC:300:LEU:HD22 | 2:EC:329:ILE:HD13 | 1.58 | 0.85 |
| 13:YA:9[E]:ASN:HA | 13:YC:7[E]:ASN:HD21 | 1.39 | 0.85 |
| 2:BJ:158:VAL:HG13 | 2:BJ:593:GLU:HG3 | 1.59 | 0.85 |
| 1:BH:63:ASN:HD22 | 1:BI:60:LEU:HB3 | 1.40 | 0.84 |
| 3:D:115:ASN:HA | 3:D:121:ALA:HA | 1.59 | 0.84 |
| 2:EC:158:VAL:HG13 | 2:EC:593:GLU:HG3 | 1.59 | 0.84 |
| 5:EI:103:ASN:N | 5:EI:127:ASN:O | 2.10 | 0.84 |
| 5:EI:215:PRO:HG3 | 5:EI:226:ASP:HB2 | 1.57 | 0.84 |
| 13:YA:7[E]:ASN:HD21 | 13:YB:9[E]:ASN:HA | 1.42 | 0.84 |
| 14:YE:125[D]:PHE:HE2 | 14:YE:134[D]:GLU:HG3 | 1.40 | 0.84 |
| 5:AC:552:VAL:HG23 | 5:AE:552:VAL:HG11 | 1.59 | 0.84 |
| 2:C:255:TYR:HB2 | 2:C:297:TYR:HB2 | 1.59 | 0.84 |
| 1:EB:98:TYR:HB2 | 1:EB:332:LYS:HG3 | 1.57 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:66:TYR:HE1 | 1:GE:21:PHE:HB2 | 1.42 | 0.84 |
| 5:HB:215:PRO:HG3 | 5:HB:226:ASP:HB2 | 1.57 | 0.84 |
| 7:HH:399:PHE:HE1 | 7:HI:401:ARG:HB3 | 1.42 | 0.84 |
| 5:HB:200:LEU:HD22 | 7:HJ:2:SER:HA | 1.58 | 0.84 |
| 14:YF:125[D]:PHE:HE2 | 14:YF:134[D]:GLU:HG3 | 1.40 | 0.84 |
| 2:BJ:255:TYR:HB2 | 2:BJ:297:TYR:HB2 | 1.59 | 0.84 |
| 5:CF:552:VAL:HG23 | 5:CH:552:VAL:HG11 | 1.59 | 0.84 |
| 13:YA:7[F]:ASN:HD21 | 13:YB:9[F]:ASN:HA | 1.42 | 0.84 |
| 14:YD:125[B]:PHE:HE2 | 14:YD:134[B]:GLU:HG3 | 1.40 | 0.84 |
| 2:Z:368:MET:HG3 | 2:Z:377:ALA:HB2 | 1.59 | 0.84 |
| 5:AD:285:LEU:HD21 | 5:AD:375:PHE:H | 1.41 | 0.84 |
| 5:AE:215:PRO:HG3 | 5:AE:226:ASP:HB2 | 1.59 | 0.84 |
| 2:C:368:MET:HG3 | 2:C:377:ALA:HB2 | 1.59 | 0.84 |
| 5:CF:103:ASN:N | 5:CF:127:ASN:O | 2.10 | 0.84 |
| 7:P:399:PHE:CE1 | 7:Q:401:ARG:HB3 | 2.12 | 0.84 |
| 13:YB:8[A]:LEU:HD21 | 13:YC:10[A]:TRP:HB3 | 1.60 | 0.84 |
| 13:YB:8[B]:LEU:HD21 | 13:YC:10[B]:TRP:HB3 | 1.60 | 0.84 |
| 2:C:580:LYS:HG2 | 2:C:581:TYR:H | 1.42 | 0.84 |
| 5:CF:200:LEU:HD22 | 7:DD:2:SER:HA | 1.60 | 0.84 |
| 2:BJ:922:ASP:HA | 5:CH:20:ARG:HD3 | 1.60 | 0.84 |
| 12:BG:211:HIS:HE1 | 12:DJ:168:ALA:H | 1.25 | 0.84 |
| 5:EI:552:VAL:HG23 | 5:FA:552:VAL:HG11 | 1.59 | 0.84 |
| 7:DC:53:THR:HG21 | 7:FG:352:ASP:HB3 | 1.59 | 0.84 |
| 1:GE:209:TRP:CD1 | 1:GE:223:ILE:HG12 | 2.13 | 0.84 |
| 5:K:111:ALA:HB2 | 5:K:117:ILE:HG23 | 1.58 | 0.84 |
| 1:Y:209:TRP:CD1 | 1:Y:223:ILE:HG12 | 2.13 | 0.84 |
| 1:X:67:ILE:HD11 | 1:Y:67:ILE:HD13 | 1.59 | 0.84 |
| 2:C:694:TYR:HD2 | 2:C:696:ARG:H | 1.26 | 0.84 |
| 5:CF:215:PRO:HG3 | 5:CF:226:ASP:HB2 | 1.57 | 0.84 |
| 5:FA:323:THR:N | 5:FA:358:VAL:O | 2.09 | 0.84 |
| 1:GE:361:GLN:HG2 | 1:GE:455:PHE:CZ | 2.13 | 0.84 |
| 5:I:215:PRO:HG3 | 5:I:226:ASP:HB2 | 1.57 | 0.84 |
| 5:I:49:TRP:O | 5:K:90:ASN:ND2 | 2.11 | 0.84 |
| 13:YA:7[B]:ASN:HD21 | 13:YB:9[B]:ASN:HA | 1.42 | 0.84 |
| 14:YD:125[F]:PHE:HE2 | 14:YD:134[F]:GLU:HG3 | 1.40 | 0.84 |
| 14:YE:125[F]:PHE:HE2 | 14:YE:134[F]:GLU:HG3 | 1.40 | 0.84 |
| 14:YF:125[B]:PHE:HE2 | 14:YF:134[B]:GLU:HG3 | 1.40 | 0.84 |
| 1:BI:194:ARG:NH2 | 1:BI:228:GLU:OE2 | 2.10 | 0.84 |
| 1:EB:194:ARG:NH2 | 1:EB:228:GLU:OE2 | 2.10 | 0.84 |
| 1:EB:361:GLN:HG2 | 1:EB:455:PHE:CZ | 2.13 | 0.84 |
| 12:W:168:ALA:H | 12:IF:211:HIS:HE1 | 1.26 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:694:TYR:HD2 | 2:BJ:696:ARG:H | 1.26 | 0.84 |
| 7:DC:399:PHE:HE1 | 7:DD:401:ARG:HB3 | 1.43 | 0.84 |
| 2:GF:580:LYS:HG2 | 2:GF:581:TYR:H | 1.42 | 0.84 |
| 1:Y:361:GLN:HG2 | 1:Y:455:PHE:CZ | 2.13 | 0.84 |
| 14:YE:125[B]:PHE:HE2 | 14:YE:134[B]:GLU:HG3 | 1.40 | 0.84 |
| 2:Z:255:TYR:HB2 | 2:Z:297:TYR:HB2 | 1.59 | 0.84 |
| 5:AE:323:THR:N | 5:AE:358:VAL:O | 2.09 | 0.84 |
| 1:GE:194:ARG:NH2 | 1:GE:228:GLU:OE2 | 2.10 | 0.84 |
| 2:GF:694:TYR:HD2 | 2:GF:696:ARG:H | 1.26 | 0.84 |
| 5:HB:552:VAL:HG23 | 5:HD:552:VAL:HG11 | 1.58 | 0.84 |
| 5:I:393:LEU:HD11 | 5:K:391:GLY:HA2 | 1.60 | 0.84 |
| 7:O:96:GLY:HA2 | 7:Q:97:LEU:HD13 | 1.60 | 0.84 |
| 13:YB:8[F]:LEU:HD21 | 13:YC:10[F]:TRP:HB3 | 1.60 | 0.84 |
| 14:YE:125[C]:PHE:HE2 | 14:YE:134[C]:GLU:HG3 | 1.40 | 0.84 |
| 14:YF:125[A]:PHE:HE2 | 14:YF:134[A]:GLU:HG3 | 1.40 | 0.84 |
| 2:Z:694:TYR:HD2 | 2:Z:696:ARG:H | 1.26 | 0.84 |
| 1:A:338:ARG:HG2 | 1:B:336:GLN:NE2 | 1.93 | 0.84 |
| 5:AD:304:ILE:HD12 | 5:AD:385:TRP:HA | 1.59 | 0.84 |
| 7:AJ:399:PHE:HE1 | 7:BA:401:ARG:HB3 | 1.43 | 0.84 |
| 5:EJ:394:LEU:HD22 | 5:FA:392:THR:HG22 | 1.58 | 0.84 |
| 14:YF:125[F]:PHE:HE2 | 14:YF:134[F]:GLU:HG3 | 1.40 | 0.84 |
| 5:AC:160:SER:HB3 | 5:AD:161:ASN:HD22 | 1.42 | 0.83 |
| 1:B:194:ARG:NH2 | 1:B:228:GLU:OE2 | 2.10 | 0.83 |
| 7:AJ:53:THR:HG21 | 7:DD:352:ASP:HB3 | 1.60 | 0.83 |
| 5:FA:496:ASP:HB3 | 5:FA:500:ALA:HB2 | 1.60 | 0.83 |
| 5:HD:496:ASP:HB3 | 5:HD:500:ALA:HB2 | 1.60 | 0.83 |
| 14:YD:125[D]:PHE:HE2 | 14:YD:134[D]:GLU:HG3 | 1.40 | 0.83 |
| 2:EC:1005:ARG:HA | 5:EI:12:ASP:HB2 | 1.60 | 0.83 |
| 2:GF:300:LEU:HD22 | 2:GF:329:ILE:HD13 | 1.58 | 0.83 |
| 5:I:160:SER:HB3 | 5:J:161:ASN:HD22 | 1.42 | 0.83 |
| 5:K:312:ARG:HG2 | 5:K:317:LEU:HA | 1.60 | 0.83 |
| 13:YB:8[E]:LEU:HD21 | 13:YC:10[E]:TRP:HB3 | 1.60 | 0.83 |
| 14:YD:125[E]:PHE:HE2 | 14:YD:134[E]:GLU:HG3 | 1.40 | 0.83 |
| 14:YE:332[D]:GLN:HE22 | 14:YF:97[D]:VAL:HG21 | 1.43 | 0.83 |
| 2:BJ:300:LEU:HD22 | 2:BJ:329:ILE:HD13 | 1.58 | 0.83 |
| 1:EB:209:TRP:CD1 | 1:EB:223:ILE:HG12 | 2.13 | 0.83 |
| 2:EC:694:TYR:HD2 | 2:EC:696:ARG:H | 1.26 | 0.83 |
| 5:EI:393:LEU:HD11 | 5:FA:391:GLY:HA2 | 1.60 | 0.83 |
| 5:EJ:191:ILE:O | 5:FA:164:ARG:NH2 | 2.10 | 0.83 |
| 5:HB:103:ASN:N | 5:HB:127:ASN:O | 2.10 | 0.83 |
| 5:HD:193:VAL:HG13 | 5:HD:199:GLU:HB3 | 1.57 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:96:GLY:HA2 | 7:HJ:97:LEU:HD13 | 1.61 | 0.83 |
| 1:X:66:TYR:HE1 | 1:Y:21:PHE:HB2 | 1.42 | 0.83 |
| 1:B:361:GLN:HG2 | 1:B:455:PHE:CZ | 2.13 | 0.83 |
| 1:BI:361:GLN:HG2 | 1:BI:455:PHE:CZ | 2.13 | 0.83 |
| 5:CH:496:ASP:HB3 | 5:CH:500:ALA:HB2 | 1.60 | 0.83 |
| 1:EA:338:ARG:HG2 | 1:EB:336:GLN:NE2 | 1.93 | 0.83 |
| 2:GF:158:VAL:HG13 | 2:GF:593:GLU:HG3 | 1.59 | 0.83 |
| 2:C:921:TRP:HE1 | 5:J:19:LEU:HA | 1.43 | 0.83 |
| 1:B:209:TRP:CD1 | 1:B:223:ILE:HG12 | 2.13 | 0.83 |
| 5:CF:362:GLU:HG3 | 5:CF:363:ASN:H | 1.44 | 0.83 |
| 2:EC:368:MET:HG3 | 2:EC:377:ALA:HB2 | 1.59 | 0.83 |
| 5:EI:362:GLU:HG3 | 5:EI:363:ASN:H | 1.44 | 0.83 |
| 5:HC:304:ILE:HD12 | 5:HC:385:TRP:HA | 1.59 | 0.83 |
| 13:YB:8[D]:LEU:HD21 | 13:YC:10[D]:TRP:HB3 | 1.60 | 0.83 |
| 5:AC:200:LEU:HD22 | 7:BA:2:SER:HA | 1.60 | 0.83 |
| 5:CG:304:ILE:HD12 | 5:CG:385:TRP:HA | 1.59 | 0.83 |
| 7:DB:399:PHE:HE1 | 7:DC:401:ARG:HB3 | 1.41 | 0.83 |
| 14:YD:360[C]:ASN:HD22 | 14:YD:360[C]:ASN:H | 1.27 | 0.83 |
| 5:CF:329:PHE:HB3 | 5:CF:332:VAL:HB | 1.61 | 0.83 |
| 3:GG:115:ASN:HA | 3:GG:121:ALA:HA | 1.59 | 0.83 |
| 14:YE:360[C]:ASN:HD22 | 14:YE:360[C]:ASN:H | 1.27 | 0.83 |
| 14:YF:360[E]:ASN:H | 14:YF:360[E]:ASN:HD22 | 1.27 | 0.83 |
| 1:BI:209:TRP:CD1 | 1:BI:223:ILE:HG12 | 2.13 | 0.83 |
| 3:ED:115:ASN:HA | 3:ED:121:ALA:HA | 1.59 | 0.83 |
| 12:GC:211:HIS:HE1 | 12:IF:168:ALA:H | 1.25 | 0.83 |
| 2:GF:164:SER:HA | 2:GF:167:ILE:HD11 | 1.60 | 0.83 |
| 5:HD:312:ARG:HG2 | 5:HD:317:LEU:HA | 1.61 | 0.83 |
| 5:AD:558:ASP:O | 5:AD:560:ASP:N | 2.12 | 0.83 |
| 5:AE:312:ARG:HG2 | 5:AE:317:LEU:HA | 1.60 | 0.83 |
| 7:AI:399:PHE:HE1 | 7:AJ:401:ARG:HB3 | 1.42 | 0.83 |
| 7:AI:49:ASP:O | 7:AI:57:ILE:N | 2.12 | 0.83 |
| 2:BJ:360:ASN:O | 2:BJ:362:LYS:N | 2.12 | 0.83 |
| 2:BJ:368:MET:HG3 | 2:BJ:377:ALA:HB2 | 1.59 | 0.83 |
| 2:GF:368:MET:HG3 | 2:GF:377:ALA:HB2 | 1.59 | 0.83 |
| 5:HD:215:PRO:HG3 | 5:HD:226:ASP:HB2 | 1.59 | 0.83 |
| 5:I:103:ASN:N | 5:I:127:ASN:O | 2.10 | 0.83 |
| 13:YA:7[D]:ASN:HD21 | 13:YB:9[D]:ASN:HA | 1.42 | 0.83 |
| 14:YD:332[A]:GLN:HE22 | 14:YE:97[A]:VAL:HG21 | 1.44 | 0.83 |
| 14:YF:360[D]:ASN:H | 14:YF:360[D]:ASN:HD22 | 1.27 | 0.83 |
| 1:A:63:ASN:HD22 | 1:B:60:LEU:HB3 | 1.41 | 0.83 |
| 5:CG:558:ASP:O | 5:CG:560:ASP:N | 2.12 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:49:TRP:O | 5:CH:90:ASN:ND2 | 2.10 | 0.83 |
| 10:U:324:THR:HG21 | 10:U:329:PHE:HA | 1.61 | 0.83 |
| 14:YD:360[E]:ASN:H | 14:YD:360[E]:ASN:HD22 | 1.27 | 0.83 |
| 2:Z:158:VAL:HG13 | 2:Z:593:GLU:HG3 | 1.59 | 0.83 |
| 6:AF:28:ASP:OD2 | 6:AG:60:HIS:NE2 | 2.11 | 0.82 |
| 2:C:164:SER:HA | 2:C:167:ILE:HD11 | 1.60 | 0.82 |
| 5:HD:359:GLU:N | 5:HD:370:HIS:O | 2.12 | 0.82 |
| 13:YA:44[B]:VAL:HG11 | 14:YF:272[B]:GLU:HB3 | 1.61 | 0.82 |
| 14:YD:360[B]:ASN:HD22 | 14:YD:360[B]:ASN:H | 1.27 | 0.82 |
| 14:YE:360[A]:ASN:H | 14:YE:360[A]:ASN:HD22 | 1.27 | 0.82 |
| 2:Z:580:LYS:HG2 | 2:Z:581:TYR:H | 1.42 | 0.82 |
| 7:DB:49:ASP:O | 7:DB:57:ILE:N | 2.12 | 0.82 |
| 2:EC:231:TYR:CZ | 2:EC:391:ARG:HD3 | 2.15 | 0.82 |
| 5:EJ:304:ILE:HD12 | 5:EJ:385:TRP:HA | 1.59 | 0.82 |
| 12:DJ:211:HIS:HE1 | 12:GC:168:ALA:H | 1.25 | 0.82 |
| 5:HC:558:ASP:O | 5:HC:560:ASP:N | 2.12 | 0.82 |
| 2:GF:922:ASP:HA | 5:HD:20:ARG:HD3 | 1.59 | 0.82 |
| 5:J:304:ILE:HD12 | 5:J:385:TRP:HA | 1.59 | 0.82 |
| 13:YB:8[C]:LEU:HD21 | 13:YC:10[C]:TRP:HB3 | 1.60 | 0.82 |
| 14:YD:360[D]:ASN:HD22 | 14:YD:360[D]:ASN:H | 1.27 | 0.82 |
| 2:Z:231:TYR:CZ | 2:Z:391:ARG:HD3 | 2.15 | 0.82 |
| 5:AC:362:GLU:HG3 | 5:AC:363:ASN:H | 1.44 | 0.82 |
| 10:BE:202:ASN:OD1 | 10:BE:349:ARG:NH2 | 2.12 | 0.82 |
| 1:BH:66:TYR:HE1 | 1:BI:21:PHE:HB2 | 1.44 | 0.82 |
| 2:BJ:164:SER:HA | 2:BJ:167:ILE:HD11 | 1.60 | 0.82 |
| 2:BJ:580:LYS:HG2 | 2:BJ:581:TYR:H | 1.42 | 0.82 |
| 5:CH:312:ARG:HG2 | 5:CH:317:LEU:HA | 1.60 | 0.82 |
| 1:EA:66:TYR:HE1 | 1:EB:21:PHE:HB2 | 1.43 | 0.82 |
| 5:EJ:558:ASP:O | 5:EJ:560:ASP:N | 2.12 | 0.82 |
| 5:FA:312:ARG:HG2 | 5:FA:317:LEU:HA | 1.61 | 0.82 |
| 13:YA:7[C]:ASN:HD21 | 13:YB:9[C]:ASN:HA | 1.43 | 0.82 |
| 13:YB:540[F]:GLY:HA3 | 13:YC:533[F]:ASN:HD22 | 1.44 | 0.82 |
| 14:YF:360[A]:ASN:H | 14:YF:360[A]:ASN:HD22 | 1.27 | 0.82 |
| 5:AC:329:PHE:HB3 | 5:AC:332:VAL:HB | 1.61 | 0.82 |
| 4:CD:113:ASN:HD22 | 4:CE:103:LEU:HD21 | 1.45 | 0.82 |
| 5:CH:202:TYR:OH | 5:CH:223:VAL:O | 1.98 | 0.82 |
| 10:DH:324:THR:HG21 | 10:DH:329:PHE:HA | 1.61 | 0.82 |
| 5:EI:329:PHE:HB3 | 5:EI:332:VAL:HB | 1.61 | 0.82 |
| 2:GF:231:TYR:CZ | 2:GF:391:ARG:HD3 | 2.15 | 0.82 |
| 14:YE:360[F]:ASN:HD22 | 14:YE:360[F]:ASN:H | 1.27 | 0.82 |
| 1:BH:338:ARG:HG2 | 1:BI:336:GLN:NE2 | 1.94 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:231:TYR:CZ | 2:BJ:391:ARG:HD3 | 2.14 | 0.82 |
| 5:FA:359:GLU:N | 5:FA:370:HIS:O | 2.12 | 0.82 |
| 5:HB:160:SER:HB3 | 5:HC:161:ASN:HD22 | 1.42 | 0.82 |
| 10:U:202:ASN:OD1 | 10:U:349:ARG:NH2 | 2.12 | 0.82 |
| 13:YA:452[C]:GLY:HA2 | 13:YC:321[C]:LYS:HD3 | 1.62 | 0.82 |
| 5:AC:49:TRP:O | 5:AE:90:ASN:ND2 | 2.11 | 0.82 |
| 10:BE:324:THR:HG21 | 10:BE:329:PHE:HA | 1.61 | 0.82 |
| 5:CF:393:LEU:HD11 | 5:CH:391:GLY:HA2 | 1.62 | 0.82 |
| 5:CF:160:SER:HB3 | 5:CG:161:ASN:HD22 | 1.42 | 0.82 |
| 5:FA:215:PRO:HG3 | 5:FA:226:ASP:HB2 | 1.59 | 0.82 |
| 5:HB:362:GLU:HG3 | 5:HB:363:ASN:H | 1.44 | 0.82 |
| 5:J:558:ASP:O | 5:J:560:ASP:N | 2.12 | 0.82 |
| 7:O:49:ASP:O | 7:O:57:ILE:N | 2.12 | 0.82 |
| 1:BI:70:PHE:HE2 | 2:BJ:686:LEU:HB3 | 1.44 | 0.82 |
| 7:DC:173:ILE:HG23 | 7:DD:173:ILE:HG12 | 1.62 | 0.82 |
| 5:K:215:PRO:HG3 | 5:K:226:ASP:HB2 | 1.59 | 0.82 |
| 5:K:496:ASP:HB3 | 5:K:500:ALA:HB2 | 1.60 | 0.82 |
| 13:YA:61[F]:ILE:HB | 13:YB:75[F]:GLY:HA2 | 1.60 | 0.82 |
| 14:YE:360[D]:ASN:HD22 | 14:YE:360[D]:ASN:H | 1.27 | 0.82 |
| 2:C:158:VAL:HG13 | 2:C:593:GLU:HG3 | 1.59 | 0.82 |
| 1:GD:338:ARG:HG2 | 1:GE:336:GLN:NE2 | 1.94 | 0.82 |
| 14:YE:360[B]:ASN:H | 14:YE:360[B]:ASN:HD22 | 1.27 | 0.82 |
| 14:YF:360[F]:ASN:HD22 | 14:YF:360[F]:ASN:H | 1.27 | 0.82 |
| 4:CD:69:LYS:NZ | 4:CE:103:LEU:O | 2.13 | 0.82 |
| 1:EB:70:PHE:HE2 | 2:EC:686:LEU:HB3 | 1.44 | 0.82 |
| 2:EC:922:ASP:HA | 5:FA:20:ARG:HD3 | 1.60 | 0.82 |
| 5:EI:200:LEU:HD22 | 7:FG:2:SER:HA | 1.61 | 0.82 |
| 14:YF:360[B]:ASN:HD22 | 14:YF:360[B]:ASN:H | 1.27 | 0.82 |
| 5:AC:393:LEU:HD11 | 5:AE:391:GLY:HA2 | 1.61 | 0.82 |
| 2:BJ:339:ASP:HB3 | 2:BJ:340:PRO:HD3 | 1.62 | 0.82 |
| 2:EC:360:ASN:O | 2:EC:362:LYS:N | 2.12 | 0.82 |
| 7:FF:173:ILE:HG23 | 7:FG:173:ILE:HG12 | 1.61 | 0.82 |
| 2:GF:360:ASN:O | 2:GF:362:LYS:N | 2.12 | 0.82 |
| 7:HI:399:PHE:HE1 | 7:HJ:401:ARG:HB3 | 1.43 | 0.82 |
| 13:YB:540[A]:GLY:HA3 | 13:YC:533[A]:ASN:HD22 | 1.45 | 0.82 |
| 14:YD:97[F]:VAL:HG21 | 14:YF:332[F]:GLN:HE22 | 1.42 | 0.82 |
| 1:A:66:TYR:HE1 | 1:B:21:PHE:HB2 | 1.43 | 0.81 |
| 5:AD:394:LEU:HD22 | 5:AE:392:THR:HG22 | 1.62 | 0.81 |
| 1:EA:63:ASN:HD22 | 1:EB:60:LEU:HB3 | 1.42 | 0.81 |
| 5:FA:202:TYR:OH | 5:FA:223:VAL:O | 1.98 | 0.81 |
| 6:FB:70:ILE:HG12 | 6:FC:73:ASN:HA | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FF:399:PHE:CE1 | 7:FG:401:ARG:HB3 | 2.14 | 0.81 |
| 1:GD:63:ASN:HD22 | 1:GE:60:LEU:HB3 | 1.43 | 0.81 |
| 10:ID:202:ASN:OD1 | 10:ID:349:ARG:NH2 | 2.12 | 0.81 |
| 13:YB:540[E]:GLY:HA3 | 13:YC:533[E]:ASN:HD22 | 1.44 | 0.81 |
| 14:YD:332[C]:GLN:HE22 | 14:YE:97[C]:VAL:HG21 | 1.43 | 0.81 |
| 14:YD:360[F]:ASN:HD22 | 14:YD:360[F]:ASN:H | 1.27 | 0.81 |
| 13:YA:44[A]:VAL:HG11 | 14:YF:272[A]:GLU:HB3 | 1.62 | 0.81 |
| 7:AI:96:GLY:HA2 | 7:BA:97:LEU:HD13 | 1.61 | 0.81 |
| 10:DH:202:ASN:OD1 | 10:DH:349:ARG:NH2 | 2.12 | 0.81 |
| 7:FE:399:PHE:HE1 | 7:FF:401:ARG:HB3 | 1.42 | 0.81 |
| 5:I:362:GLU:HG3 | 5:I:363:ASN:H | 1.44 | 0.81 |
| 5:I:552:VAL:HG23 | 5:K:552:VAL:HG11 | 1.60 | 0.81 |
| 14:YD:332[B]:GLN:HE22 | 14:YE:97[B]:VAL:HG21 | 1.43 | 0.81 |
| 2:Z:360:ASN:O | 2:Z:362:LYS:N | 2.12 | 0.81 |
| 2:C:360:ASN:O | 2:C:362:LYS:N | 2.12 | 0.81 |
| 2:EC:164:SER:HA | 2:EC:167:ILE:HD11 | 1.60 | 0.81 |
| 7:FF:212:PRO:HB3 | 7:FG:199:VAL:HA | 1.62 | 0.81 |
| 5:HC:117:ILE:HA | 5:HC:143:TRP:HB2 | 1.63 | 0.81 |
| 5:AE:359:GLU:N | 5:AE:370:HIS:O | 2.12 | 0.81 |
| 5:CH:215:PRO:HG3 | 5:CH:226:ASP:HB2 | 1.59 | 0.81 |
| 7:FE:49:ASP:O | 7:FE:57:ILE:N | 2.12 | 0.81 |
| 7:FE:98:THR:HG1 | 7:FG:100:TYR:HH | 0.81 | 0.81 |
| 7:FF:144:ILE:HG21 | 7:FG:156:ASP:HB3 | 1.62 | 0.81 |
| 5:HC:394:LEU:HD22 | 5:HD:392:THR:HG22 | 1.62 | 0.81 |
| 5:K:359:GLU:N | 5:K:370:HIS:O | 2.12 | 0.81 |
| 5:J:394:LEU:HD22 | 5:K:392:THR:HG22 | 1.62 | 0.81 |
| 13:YA:61[C]:ILE:HG21 | 13:YB:59[C]:GLN:HA | 1.62 | 0.81 |
| 13:YA:452[D]:GLY:HA2 | 13:YC:321[D]:LYS:HD3 | 1.62 | 0.81 |
| 13:YC:89[E]:LYS:HE2 | 13:YC:89[E]:LYS:H | 1.46 | 0.81 |
| 13:YA:10[D]:TRP:HB3 | 13:YC:8[D]:LEU:HD21 | 1.62 | 0.81 |
| 14:YF:360[C]:ASN:HD22 | 14:YF:360[C]:ASN:H | 1.27 | 0.81 |
| 5:AE:496:ASP:HB3 | 5:AE:500:ALA:HB2 | 1.60 | 0.81 |
| 1:B:70:PHE:HE2 | 2:C:686:LEU:HB3 | 1.44 | 0.81 |
| 7:AJ:173:ILE:HG23 | 7:BA:173:ILE:HG12 | 1.62 | 0.81 |
| 2:C:231:TYR:CZ | 2:C:391:ARG:HD3 | 2.15 | 0.81 |
| 5:EI:191:ILE:O | 5:EJ:164:ARG:NH1 | 2.14 | 0.81 |
| 4:G:113:ASN:HD22 | 4:H:103:LEU:HD21 | 1.44 | 0.81 |
| 14:YE:360[E]:ASN:HD22 | 14:YE:360[E]:ASN:H | 1.27 | 0.81 |
| 2:Z:339:ASP:HB3 | 2:Z:340:PRO:HD3 | 1.62 | 0.81 |
| 5:AC:160:SER:OG | 5:AC:248:MET:O | 1.98 | 0.81 |
| 5:AD:312:ARG:HB2 | 5:AD:382:ASN:HB2 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:329:PHE:HB3 | 5:AE:332:VAL:HB | 1.62 | 0.81 |
| 7:FE:147:LEU:HD23 | 7:FE:164:LYS:HG3 | 1.63 | 0.81 |
| 5:HD:202:TYR:OH | 5:HD:223:VAL:O | 1.98 | 0.81 |
| 5:I:160:SER:OG | 5:I:248:MET:O | 1.98 | 0.81 |
| 7:P:399:PHE:HE1 | 7:Q:401:ARG:HB3 | 1.44 | 0.81 |
| 13:YA:10[B]:TRP:HB3 | 13:YC:8[B]:LEU:HD21 | 1.62 | 0.81 |
| 13:YA:7[A]:ASN:HD21 | 13:YB:9[A]:ASN:HA | 1.42 | 0.81 |
| 13:YC:89[D]:LYS:HE2 | 13:YC:89[D]:LYS:H | 1.46 | 0.81 |
| 2:BJ:992:PRO:O | 5:CH:19:LEU:N | 2.13 | 0.81 |
| 5:CG:191:ILE:O | 5:CH:164:ARG:NH2 | 2.14 | 0.81 |
| 5:HB:202:TYR:OH | 5:HB:223:VAL:O | 1.98 | 0.81 |
| 7:HH:147:LEU:HD23 | 7:HH:164:LYS:HG3 | 1.63 | 0.81 |
| 5:K:103:ASN:N | 5:K:127:ASN:O | 2.14 | 0.81 |
| 13:YA:10[A]:TRP:HB3 | 13:YC:8[A]:LEU:HD21 | 1.62 | 0.81 |
| 13:YA:89[D]:LYS:HE2 | 13:YA:89[D]:LYS:H | 1.46 | 0.81 |
| 13:YA:89[C]:LYS:H | 13:YA:89[C]:LYS:HE2 | 1.46 | 0.81 |
| 13:YB:89[A]:LYS:HE2 | 13:YB:89[A]:LYS:H | 1.46 | 0.81 |
| 13:YB:89[B]:LYS:H | 13:YB:89[B]:LYS:HE2 | 1.46 | 0.81 |
| 14:YE:332[C]:GLN:HE22 | 14:YF:97[C]:VAL:HG21 | 1.44 | 0.81 |
| 2:Z:164:SER:HA | 2:Z:167:ILE:HD11 | 1.60 | 0.81 |
| 1:A:84:ASN:ND2 | 11:V:14:LYS:O | 2.12 | 0.81 |
| 7:AI:147:LEU:HD23 | 7:AI:164:LYS:HG3 | 1.63 | 0.81 |
| 5:CH:353:HIS:HB2 | 7:HJ:478:ASP:HB3 | 1.63 | 0.81 |
| 7:DB:147:LEU:HD23 | 7:DB:164:LYS:HG3 | 1.63 | 0.81 |
| 5:HD:329:PHE:HB3 | 5:HD:332:VAL:HB | 1.62 | 0.81 |
| 13:YA:10[F]:TRP:HB3 | 13:YC:8[F]:LEU:HD21 | 1.63 | 0.81 |
| 13:YA:10[E]:TRP:HB3 | 13:YC:8[E]:LEU:HD21 | 1.63 | 0.81 |
| 5:AE:202:TYR:OH | 5:AE:223:VAL:O | 1.98 | 0.81 |
| 7:FE:96:GLY:HA2 | 7:FG:97:LEU:HD13 | 1.63 | 0.81 |
| 5:HB:191:ILE:O | 5:HC:164:ARG:NH1 | 2.14 | 0.81 |
| 5:HB:329:PHE:HB3 | 5:HB:332:VAL:HB | 1.61 | 0.81 |
| 7:HI:144:ILE:HG21 | 7:HJ:156:ASP:HB3 | 1.63 | 0.81 |
| 5:I:200:LEU:HD22 | 7:Q:2:SER:HA | 1.63 | 0.81 |
| 7:O:147:LEU:HD23 | 7:O:164:LYS:HG3 | 1.63 | 0.81 |
| 13:YA:89[B]:LYS:H | 13:YA:89[B]:LYS:HE2 | 1.46 | 0.81 |
| 13:YA:76[F]:PRO:HG3 | 13:YA:96[F]:VAL:HB | 1.62 | 0.81 |
| 14:YD:360[A]:ASN:HD22 | 14:YD:360[A]:ASN:H | 1.27 | 0.81 |
| 7:BA:49:ASP:O | 7:BA:56:GLY:HA3 | 1.81 | 0.81 |
| 9:BD:20:ASN:HA | 1:BI:311:VAL:HG11 | 1.61 | 0.81 |
| 2:GF:504:GLN:NE2 | 2:GF:505:PRO:HD2 | 1.96 | 0.81 |
| 5:HD:103:ASN:N | 5:HD:127:ASN:O | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:329:PHE:HB3 | 5:I:332:VAL:HB | 1.61 | 0.81 |
| 7:P:173:ILE:HG23 | 7:Q:173:ILE:HG12 | 1.62 | 0.81 |
| 5:CF:202:TYR:OH | 5:CF:223:VAL:O | 1.98 | 0.81 |
| 7:DD:49:ASP:O | 7:DD:56:GLY:HA3 | 1.82 | 0.81 |
| 10:GA:202:ASN:OD1 | 10:GA:349:ARG:NH2 | 2.12 | 0.81 |
| 9:FJ:20:ASN:HA | 1:GE:311:VAL:HG11 | 1.62 | 0.81 |
| 7:HH:98:THR:HG1 | 7:HJ:100:TYR:HH | 0.81 | 0.81 |
| 7:P:212:PRO:HB3 | 7:Q:199:VAL:HA | 1.63 | 0.81 |
| 13:YB:89[D]:LYS:H | 13:YB:89[D]:LYS:HE2 | 1.46 | 0.81 |
| 13:YB:89[E]:LYS:H | 13:YB:89[E]:LYS:HE2 | 1.46 | 0.81 |
| 13:YB:89[F]:LYS:HE2 | 13:YB:89[F]:LYS:H | 1.46 | 0.81 |
| 13:YC:89[F]:LYS:HE2 | 13:YC:89[F]:LYS:H | 1.46 | 0.81 |
| 14:YD:97[B]:VAL:HG21 | 14:YF:332[B]:GLN:HE22 | 1.45 | 0.81 |
| 5:AE:339:GLU:HB2 | 6:AF:171:TYR:HB2 | 1.63 | 0.80 |
| 5:HC:90:ASN:ND2 | 5:HD:49:TRP:O | 2.12 | 0.80 |
| 7:HI:212:PRO:HB3 | 7:HJ:199:VAL:HA | 1.63 | 0.80 |
| 1:Y:555:ILE:HB | 1:Y:592:ILE:HD11 | 1.63 | 0.80 |
| 13:YA:89[A]:LYS:HE2 | 13:YA:89[A]:LYS:H | 1.46 | 0.80 |
| 13:YB:540[B]:GLY:HA3 | 13:YC:533[B]:ASN:HD22 | 1.45 | 0.80 |
| 13:YC:89[B]:LYS:HE2 | 13:YC:89[B]:LYS:H | 1.46 | 0.80 |
| 13:YA:10[C]:TRP:HB3 | 13:YC:8[C]:LEU:HD21 | 1.63 | 0.80 |
| 5:CG:394:LEU:HD22 | 5:CH:392:THR:HG22 | 1.62 | 0.80 |
| 2:EC:504:GLN:NE2 | 2:EC:505:PRO:HD2 | 1.96 | 0.80 |
| 5:EJ:90:ASN:ND2 | 5:FA:49:TRP:O | 2.13 | 0.80 |
| 2:GF:947:VAL:HA | 3:GG:118:PRO:HB2 | 1.64 | 0.80 |
| 7:HH:49:ASP:O | 7:HH:57:ILE:N | 2.12 | 0.80 |
| 6:L:86:ASP:OD2 | 6:L:180:GLN:NE2 | 2.14 | 0.80 |
| 7:P:144:ILE:HG21 | 7:Q:156:ASP:HB3 | 1.63 | 0.80 |
| 1:Y:70:PHE:HE2 | 2:Z:686:LEU:HB3 | 1.44 | 0.80 |
| 13:YA:89[E]:LYS:H | 13:YA:89[E]:LYS:HE2 | 1.46 | 0.80 |
| 13:YB:540[C]:GLY:HA3 | 13:YC:533[C]:ASN:HD22 | 1.44 | 0.80 |
| 2:Z:504:GLN:NE2 | 2:Z:505:PRO:HD2 | 1.96 | 0.80 |
| 3:D:202:ARG:HB3 | 3:D:209:VAL:HG21 | 1.63 | 0.80 |
| 2:EC:333:ASN:HB2 | 4:EF:18:ALA:HA | 1.62 | 0.80 |
| 5:FA:329:PHE:HB3 | 5:FA:332:VAL:HB | 1.62 | 0.80 |
| 6:FB:86:ASP:OD2 | 6:FB:180:GLN:NE2 | 2.14 | 0.80 |
| 7:FG:151:LEU:HB2 | 7:FG:168:LEU:HD13 | 1.63 | 0.80 |
| 8:DF:56:ARG:HD3 | 8:FI:64:ARG:HD3 | 1.62 | 0.80 |
| 10:GA:324:THR:HG21 | 10:GA:329:PHE:HA | 1.61 | 0.80 |
| 2:GF:992:PRO:O | 5:HD:19:LEU:N | 2.14 | 0.80 |
| 6:HE:86:ASP:OD2 | 6:HE:180:GLN:NE2 | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:89[F]:LYS:H | 13:YA:89[F]:LYS:HE2 | 1.46 | 0.80 |
| 13:YB:61[E]:ILE:HG23 | 13:YC:60[E]:PRO:HD3 | 1.62 | 0.80 |
| 13:YC:89[A]:LYS:H | 13:YC:89[A]:LYS:HE2 | 1.46 | 0.80 |
| 2:C:18:ALA:HA | 2:Z:333:ASN:HB2 | 170.83 | 0.80 |
| 6:AH:86:ASP:OD2 | 6:AH:180:GLN:NE2 | 2.14 | 0.80 |
| 2:BJ:1005:ARG:HA | 5:CF:12:ASP:HB2 | 1.64 | 0.80 |
| 2:C:992:PRO:O | 5:K:19:LEU:N | 2.14 | 0.80 |
| 6:CI:86:ASP:OD2 | 6:CI:180:GLN:NE2 | 2.14 | 0.80 |
| 7:DC:144:ILE:HG21 | 7:DD:156:ASP:HB3 | 1.63 | 0.80 |
| 2:EC:339:ASP:HB3 | 2:EC:340:PRO:HD3 | 1.62 | 0.80 |
| 5:EJ:117:ILE:HA | 5:EJ:143:TRP:HB2 | 1.63 | 0.80 |
| 1:GE:70:PHE:HE2 | 2:GF:686:LEU:HB3 | 1.45 | 0.80 |
| 6:M:86:ASP:OD2 | 6:M:180:GLN:NE2 | 2.14 | 0.80 |
| 13:YB:540[D]:GLY:HA3 | 13:YC:533[D]:ASN:HD22 | 1.45 | 0.80 |
| 13:YC:89[C]:LYS:H | 13:YC:89[C]:LYS:HE2 | 1.46 | 0.80 |
| 6:AF:86:ASP:OD2 | 6:AF:180:GLN:NE2 | 2.14 | 0.80 |
| 7:AJ:212:PRO:HB3 | 7:BA:199:VAL:HA | 1.63 | 0.80 |
| 2:C:504:GLN:NE2 | 2:C:505:PRO:HD2 | 1.96 | 0.80 |
| 5:CF:191:ILE:O | 5:CG:164:ARG:NH1 | 2.14 | 0.80 |
| 5:CH:329:PHE:HB3 | 5:CH:332:VAL:HB | 1.62 | 0.80 |
| 7:DC:162:PRO:O | 7:DC:166:GLN:N | 2.14 | 0.80 |
| 5:EI:202:TYR:OH | 5:EI:223:VAL:O | 1.98 | 0.80 |
| 5:EI:49:TRP:O | 5:FA:90:ASN:ND2 | 2.11 | 0.80 |
| 8:S:64:ARG:HD3 | 8:IB:56:ARG:HD3 | 1.64 | 0.80 |
| 5:K:202:TYR:OH | 5:K:223:VAL:O | 1.98 | 0.80 |
| 13:YB:89[C]:LYS:HE2 | 13:YB:89[C]:LYS:H | 1.46 | 0.80 |
| 13:YC:44[D]:VAL:HG11 | 14:YE:272[D]:GLU:HB3 | 1.63 | 0.80 |
| 14:YD:332[D]:GLN:HE22 | 14:YE:97[D]:VAL:HG21 | 1.45 | 0.80 |
| 7:AJ:144:ILE:HG21 | 7:BA:156:ASP:HB3 | 1.63 | 0.80 |
| 5:CH:103:ASN:N | 5:CH:127:ASN:O | 2.14 | 0.80 |
| 1:EB:346:ASP:OD1 | 1:EB:347:THR:N | 2.15 | 0.80 |
| 4:EF:103:LEU:O | 4:EH:69:LYS:NZ | 2.15 | 0.80 |
| 5:HB:160:SER:OG | 5:HB:248:MET:O | 1.98 | 0.80 |
| 6:HF:86:ASP:OD2 | 6:HF:180:GLN:NE2 | 2.14 | 0.80 |
| 13:YB:382[B]:SER:OG | 13:YB:423[B]:GLU:OE2 | 2.00 | 0.80 |
| 2:BJ:504:GLN:NE2 | 2:BJ:505:PRO:HD2 | 1.96 | 0.80 |
| 2:EC:921:TRP:HE1 | 5:EJ:19:LEU:HA | 1.45 | 0.80 |
| 13:YA:382[E]:SER:OG | 13:YA:423[E]:GLU:OE2 | 2.00 | 0.80 |
| 13:YC:382[A]:SER:OG | 13:YC:423[A]:GLU:OE2 | 2.00 | 0.80 |
| 13:YA:75[F]:GLY:HA2 | 13:YC:61[F]:ILE:HB | 1.64 | 0.80 |
| 2:Z:206:GLN:OE1 | 2:Z:206:GLN:N | 2.15 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:202:TYR:OH | 5:AC:223:VAL:O | 1.98 | 0.80 |
| 1:BH:374:ILE:HB | 1:BH:408:ILE:HG12 | 1.64 | 0.80 |
| 1:BI:346:ASP:OD1 | 1:BI:347:THR:N | 2.15 | 0.80 |
| 2:BJ:947:VAL:HA | 3:CA:118:PRO:HB2 | 1.63 | 0.80 |
| 5:EI:160:SER:HB3 | 5:EJ:161:ASN:HD22 | 1.44 | 0.80 |
| 5:EJ:312:ARG:HB2 | 5:EJ:382:ASN:HB2 | 1.62 | 0.80 |
| 7:FF:162:PRO:O | 7:FF:166:GLN:N | 2.14 | 0.80 |
| 5:AE:353:HIS:HB2 | 7:FG:478:ASP:HB3 | 1.63 | 0.80 |
| 1:GE:472:ASP:O | 1:GE:473:HIS:ND1 | 2.15 | 0.80 |
| 2:GF:366:TYR:HB2 | 2:GF:380:ILE:HD11 | 1.64 | 0.80 |
| 5:HC:312:ARG:HB2 | 5:HC:382:ASN:HB2 | 1.62 | 0.80 |
| 13:YA:382[D]:SER:OG | 13:YA:423[D]:GLU:OE2 | 2.00 | 0.80 |
| 13:YC:44[C]:VAL:HG11 | 14:YE:272[C]:GLU:HB3 | 1.64 | 0.80 |
| 2:C:148:ASN:OD1 | 2:C:149:GLU:N | 2.15 | 0.80 |
| 6:CJ:86:ASP:OD2 | 6:CJ:180:GLN:NE2 | 2.15 | 0.80 |
| 7:DC:212:PRO:HB3 | 7:DD:199:VAL:HA | 1.63 | 0.80 |
| 7:DB:96:GLY:HA2 | 7:DD:97:LEU:HD13 | 1.62 | 0.80 |
| 2:GF:148:ASN:OD1 | 2:GF:149:GLU:N | 2.15 | 0.80 |
| 2:GF:921:TRP:HE1 | 5:HC:19:LEU:HA | 1.46 | 0.80 |
| 12:IF:163:ARG:HG2 | 12:IF:238:THR:HG22 | 1.64 | 0.80 |
| 13:YB:382[A]:SER:OG | 13:YB:423[A]:GLU:OE2 | 2.00 | 0.80 |
| 13:YA:452[F]:GLY:HA2 | 13:YC:321[F]:LYS:HD3 | 1.62 | 0.80 |
| 13:YC:382[E]:SER:OG | 13:YC:423[E]:GLU:OE2 | 2.00 | 0.80 |
| 1:A:492:TYR:HA | 1:A:606:ILE:HD12 | 1.64 | 0.80 |
| 5:AC:191:ILE:O | 5:AD:164:ARG:NH1 | 2.15 | 0.80 |
| 5:AD:90:ASN:ND2 | 5:AE:49:TRP:O | 2.15 | 0.80 |
| 7:BA:151:LEU:HB2 | 7:BA:168:LEU:HD13 | 1.63 | 0.80 |
| 7:AJ:291:ARG:NH2 | 7:BA:269:ALA:O | 2.15 | 0.80 |
| 5:CF:160:SER:OG | 5:CF:248:MET:O | 1.98 | 0.80 |
| 12:BG:142:ASN:ND2 | 10:DH:210:ASP:O | 2.15 | 0.80 |
| 2:EC:366:TYR:HB2 | 2:EC:380:ILE:HD11 | 1.64 | 0.80 |
| 3:ED:202:ARG:HB3 | 3:ED:209:VAL:HG21 | 1.63 | 0.80 |
| 2:GF:339:ASP:HB3 | 2:GF:340:PRO:HD3 | 1.62 | 0.80 |
| 6:HG:86:ASP:OD2 | 6:HG:180:GLN:NE2 | 2.14 | 0.80 |
| 7:HI:173:ILE:HG23 | 7:HJ:173:ILE:HG12 | 1.62 | 0.80 |
| 5:I:202:TYR:OH | 5:I:223:VAL:O | 1.98 | 0.80 |
| 10:ID:324:THR:HG21 | 10:ID:329:PHE:HA | 1.61 | 0.80 |
| 13:YA:44[E]:VAL:HG11 | 14:YF:272[E]:GLU:HB3 | 1.62 | 0.80 |
| 13:YC:172[E]:PRO:HB3 | 13:YC:336[E]:LEU:HD22 | 1.64 | 0.80 |
| 14:YD:332[F]:GLN:HE22 | 14:YE:97[F]:VAL:HG21 | 1.47 | 0.80 |
| 6:DA:86:ASP:OD2 | 6:DA:180:GLN:NE2 | 2.14 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:148:ASN:OD1 | 2:EC:149:GLU:N | 2.15 | 0.79 |
| 5:J:90:ASN:ND2 | 5:K:49:TRP:O | 2.15 | 0.79 |
| 1:Y:346:ASP:OD1 | 1:Y:347:THR:N | 2.15 | 0.79 |
| 6:AG:86:ASP:OD2 | 6:AG:180:GLN:NE2 | 2.14 | 0.79 |
| 7:AJ:162:PRO:O | 7:AJ:166:GLN:N | 2.14 | 0.79 |
| 8:BC:56:ARG:HD3 | 8:DF:64:ARG:HD3 | 1.63 | 0.79 |
| 5:CG:359:GLU:HB3 | 5:CG:370:HIS:HB3 | 1.64 | 0.79 |
| 5:CH:363:ASN:HB2 | 7:HJ:473:LYS:HG2 | 1.64 | 0.79 |
| 7:FF:399:PHE:HE1 | 7:FG:401:ARG:HB3 | 1.47 | 0.79 |
| 4:G:69:LYS:NZ | 4:H:103:LEU:O | 2.13 | 0.79 |
| 5:HB:507:ASP:OD1 | 5:HB:511:ASN:N | 2.15 | 0.79 |
| 7:Q:151:LEU:HB2 | 7:Q:168:LEU:HD13 | 1.63 | 0.79 |
| 1:X:374:ILE:HB | 1:X:408:ILE:HG12 | 1.64 | 0.79 |
| 13:YA:452[A]:GLY:HA2 | 13:YC:321[A]:LYS:HD3 | 1.62 | 0.79 |
| 13:YA:452[B]:GLY:HA2 | 13:YC:321[B]:LYS:HD3 | 1.63 | 0.79 |
| 2:BJ:148:ASN:OD1 | 2:BJ:149:GLU:N | 2.15 | 0.79 |
| 2:C:1005:ARG:HA | 5:I:12:ASP:HB2 | 1.63 | 0.79 |
| 5:CH:359:GLU:N | 5:CH:370:HIS:O | 2.12 | 0.79 |
| 7:DD:151:LEU:HB2 | 7:DD:168:LEU:HD13 | 1.63 | 0.79 |
| 5:EI:160:SER:OG | 5:EI:248:MET:O | 1.98 | 0.79 |
| 13:YA:172[B]:PRO:HB3 | 13:YA:336[B]:LEU:HD22 | 1.65 | 0.79 |
| 13:YA:44[F]:VAL:HG11 | 14:YF:272[F]:GLU:HB3 | 1.63 | 0.79 |
| 13:YB:382[C]:SER:OG | 13:YB:423[C]:GLU:OE2 | 2.01 | 0.79 |
| 13:YC:382[F]:SER:OG | 13:YC:423[F]:GLU:OE2 | 2.01 | 0.79 |
| 1:B:555:ILE:HB | 1:B:592:ILE:HD11 | 1.63 | 0.79 |
| 1:BI:555:ILE:HB | 1:BI:592:ILE:HD11 | 1.63 | 0.79 |
| 2:C:339:ASP:HB3 | 2:C:340:PRO:HD3 | 1.62 | 0.79 |
| 2:C:947:VAL:HA | 3:D:118:PRO:HB2 | 1.64 | 0.79 |
| 2:EC:947:VAL:HA | 3:ED:118:PRO:HB2 | 1.65 | 0.79 |
| 5:EJ:359:GLU:HB3 | 5:EJ:370:HIS:HB3 | 1.64 | 0.79 |
| 5:FA:260:ARG:O | 5:FA:261:ARG:NH1 | 2.16 | 0.79 |
| 7:FG:49:ASP:O | 7:FG:56:GLY:HA3 | 1.82 | 0.79 |
| 1:GE:346:ASP:OD1 | 1:GE:347:THR:N | 2.15 | 0.79 |
| 12:W:163:ARG:HG2 | 12:W:238:THR:HG22 | 1.64 | 0.79 |
| 1:Y:472:ASP:O | 1:Y:473:HIS:ND1 | 2.15 | 0.79 |
| 13:YB:172[B]:PRO:HB3 | 13:YB:336[B]:LEU:HD22 | 1.64 | 0.79 |
| 14:YE:332[B]:GLN:HE22 | 14:YF:97[B]:VAL:HG21 | 1.47 | 0.79 |
| 13:YA:44[D]:VAL:HG11 | 14:YF:272[D]:GLU:HB3 | 1.62 | 0.79 |
| 5:AD:191:ILE:O | 5:AE:164:ARG:NH2 | 2.15 | 0.79 |
| 1:B:325:ILE:O | 1:B:329:GLY:N | 2.15 | 0.79 |
| 2:C:206:GLN:OE1 | 2:C:206:GLN:N | 2.15 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:922:ASP:HA | 5:K:20:ARG:HD3 | 1.63 | 0.79 |
| 12:GC:211:HIS:CE1 | 12:IF:168:ALA:H | 2.01 | 0.79 |
| 1:GE:325:ILE:O | 1:GE:329:GLY:N | 2.15 | 0.79 |
| 13:YA:382[C]:SER:OG | 13:YA:423[C]:GLU:OE2 | 2.01 | 0.79 |
| 13:YB:172[A]:PRO:HB3 | 13:YB:336[A]:LEU:HD22 | 1.65 | 0.79 |
| 13:YC:382[B]:SER:OG | 13:YC:423[B]:GLU:OE2 | 2.00 | 0.79 |
| 13:YC:76[F]:PRO:HG3 | 13:YC:96[F]:VAL:HB | 1.62 | 0.79 |
| 13:YC:44[F]:VAL:HG11 | 14:YE:272[F]:GLU:HB3 | 1.63 | 0.79 |
| 13:YA:44[C]:VAL:HG11 | 14:YF:272[C]:GLU:HB3 | 1.61 | 0.79 |
| 1:BI:472:ASP:O | 1:BI:473:HIS:ND1 | 2.15 | 0.79 |
| 1:EB:555:ILE:HB | 1:EB:592:ILE:HD11 | 1.63 | 0.79 |
| 3:GG:202:ARG:HB3 | 3:GG:209:VAL:HG21 | 1.63 | 0.79 |
| 7:HI:78:PRO:HB3 | 7:HJ:66:VAL:HA | 1.65 | 0.79 |
| 7:HJ:49:ASP:O | 7:HJ:56:GLY:HA3 | 1.81 | 0.79 |
| 5:J:191:ILE:O | 5:K:164:ARG:NH2 | 2.14 | 0.79 |
| 7:P:291:ARG:NH2 | 7:Q:269:ALA:O | 2.15 | 0.79 |
| 7:Q:49:ASP:O | 7:Q:56:GLY:HA3 | 1.81 | 0.79 |
| 13:YA:172[C]:PRO:HB3 | 13:YA:336[C]:LEU:HD22 | 1.65 | 0.79 |
| 2:Z:981:GLN:HG2 | 2:Z:982:LEU:H | 1.48 | 0.79 |
| 1:B:536:TYR:OH | 1:B:562:ASP:OD2 | 2.01 | 0.79 |
| 7:BA:101:SER:O | 7:BA:120:LYS:NZ | 2.16 | 0.79 |
| 5:CH:260:ARG:O | 5:CH:261:ARG:NH1 | 2.16 | 0.79 |
| 7:DB:473:LYS:HD2 | 7:DD:473:LYS:HB3 | 1.65 | 0.79 |
| 7:Q:473:LYS:HG2 | 5:FA:363:ASN:HB2 | 1.65 | 0.79 |
| 7:FE:401:ARG:HB3 | 7:FG:399:PHE:CE1 | 2.17 | 0.79 |
| 2:GF:1005:ARG:HA | 5:HB:12:ASP:HB2 | 1.65 | 0.79 |
| 7:HI:99:ARG:HD3 | 7:HI:111:ASN:HD21 | 1.48 | 0.79 |
| 5:CG:412:PRO:HG3 | 7:HI:457:LEU:HD21 | 1.63 | 0.79 |
| 5:AD:117:ILE:HA | 5:AD:143:TRP:HB2 | 1.63 | 0.79 |
| 5:AD:33:LEU:HA | 5:AE:43:PRO:HG3 | 1.63 | 0.79 |
| 7:DC:291:ARG:NH2 | 7:DD:269:ALA:O | 2.15 | 0.79 |
| 1:EB:472:ASP:O | 1:EB:473:HIS:ND1 | 2.15 | 0.79 |
| 1:GE:536:TYR:OH | 1:GE:562:ASP:OD2 | 2.01 | 0.79 |
| 10:U:210:ASP:O | 12:IF:142:ASN:ND2 | 2.16 | 0.79 |
| 5:K:329:PHE:HB3 | 5:K:332:VAL:HB | 1.62 | 0.79 |
| 7:P:99:ARG:HD3 | 7:P:111:ASN:HD21 | 1.48 | 0.79 |
| 13:YA:382[B]:SER:OG | 13:YA:423[B]:GLU:OE2 | 2.00 | 0.79 |
| 13:YB:172[F]:PRO:HB3 | 13:YB:336[F]:LEU:HD22 | 1.65 | 0.79 |
| 13:YB:382[D]:SER:OG | 13:YB:423[D]:GLU:OE2 | 2.00 | 0.79 |
| 13:YC:172[D]:PRO:HB3 | 13:YC:336[D]:LEU:HD22 | 1.65 | 0.79 |
| 1:A:374:ILE:HB | 1:A:408:ILE:HG12 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:45:ASP:O | 1:B:47:ASP:N | 2.16 | 0.79 |
| 12:BG:163:ARG:HG2 | 12:BG:238:THR:HG22 | 1.64 | 0.79 |
| 1:BH:492:TYR:HA | 1:BH:606:ILE:HD12 | 1.64 | 0.79 |
| 2:BJ:981:GLN:HG2 | 2:BJ:982:LEU:H | 1.48 | 0.79 |
| 1:EA:374:ILE:HB | 1:EA:408:ILE:HG12 | 1.64 | 0.79 |
| 2:EC:206:GLN:OE1 | 2:EC:206:GLN:N | 2.15 | 0.79 |
| 2:EC:992:PRO:O | 5:FA:19:LEU:N | 2.16 | 0.79 |
| 1:GD:492:TYR:HA | 1:GD:606:ILE:HD12 | 1.64 | 0.79 |
| 5:HC:339:GLU:HB2 | 6:HG:171:TYR:HB2 | 1.63 | 0.79 |
| 5:I:191:ILE:O | 5:J:164:ARG:NH1 | 2.15 | 0.79 |
| 5:J:117:ILE:HA | 5:J:143:TRP:HB2 | 1.63 | 0.79 |
| 13:YA:382[F]:SER:OG | 13:YA:423[F]:GLU:OE2 | 2.01 | 0.79 |
| 13:YC:382[D]:SER:OG | 13:YC:423[D]:GLU:OE2 | 2.00 | 0.79 |
| 2:Z:148:ASN:OD1 | 2:Z:149:GLU:N | 2.15 | 0.79 |
| 4:AA:69:LYS:NZ | 4:AB:103:LEU:O | 2.16 | 0.79 |
| 12:BG:211:HIS:CE1 | 12:DJ:168:ALA:H | 2.01 | 0.79 |
| 7:DC:99:ARG:HD3 | 7:DC:111:ASN:HD21 | 1.48 | 0.79 |
| 6:FC:86:ASP:OD2 | 6:FC:180:GLN:NE2 | 2.14 | 0.79 |
| 7:FF:99:ARG:HD3 | 7:FF:111:ASN:HD21 | 1.48 | 0.79 |
| 7:FE:13:SER:HB2 | 7:FF:18:PHE:HA | 1.64 | 0.79 |
| 5:J:312:ARG:HB2 | 5:J:382:ASN:HB2 | 1.62 | 0.79 |
| 6:N:86:ASP:OD2 | 6:N:180:GLN:NE2 | 2.14 | 0.79 |
| 13:YC:44[E]:VAL:HG11 | 14:YE:272[E]:GLU:HB3 | 1.62 | 0.79 |
| 2:BJ:206:GLN:N | 2:BJ:206:GLN:OE1 | 2.15 | 0.78 |
| 5:FA:103:ASN:N | 5:FA:127:ASN:O | 2.14 | 0.78 |
| 5:FA:339:GLU:HB2 | 6:FB:171:TYR:HB2 | 1.65 | 0.78 |
| 6:FD:86:ASP:OD2 | 6:FD:180:GLN:NE2 | 2.14 | 0.78 |
| 5:AE:363:ASN:HB2 | 7:FG:473:LYS:HG2 | 1.65 | 0.78 |
| 5:HD:260:ARG:O | 5:HD:261:ARG:NH1 | 2.16 | 0.78 |
| 2:Z:304:VAL:HG13 | 2:Z:327:ARG:HH12 | 1.48 | 0.78 |
| 1:BI:45:ASP:O | 1:BI:47:ASP:N | 2.16 | 0.78 |
| 5:CG:117:ILE:HA | 5:CG:143:TRP:HB2 | 1.63 | 0.78 |
| 5:CG:312:ARG:HB2 | 5:CG:382:ASN:HB2 | 1.62 | 0.78 |
| 7:Q:478:ASP:HB3 | 5:FA:353:HIS:HB2 | 1.65 | 0.78 |
| 7:HI:291:ARG:NH2 | 7:HJ:269:ALA:O | 2.15 | 0.78 |
| 13:YA:172[E]:PRO:HB3 | 13:YA:336[E]:LEU:HD22 | 1.65 | 0.78 |
| 13:YB:382[E]:SER:OG | 13:YB:423[E]:GLU:OE2 | 2.00 | 0.78 |
| 13:YB:382[F]:SER:OG | 13:YB:423[F]:GLU:OE2 | 2.01 | 0.78 |
| 13:YC:172[F]:PRO:HB3 | 13:YC:336[F]:LEU:HD22 | 1.65 | 0.78 |
| 13:YA:452[E]:GLY:HA2 | 13:YC:321[E]:LYS:HD3 | 1.63 | 0.78 |
| 7:AI:386:ASN:OD1 | 7:AI:389:ASN:N | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:536:TYR:OH | 1:BI:562:ASP:OD2 | 2.01 | 0.78 |
| 12:GC:163:ARG:HG2 | 12:GC:238:THR:HG22 | 1.64 | 0.78 |
| 4:GI:103:LEU:O | 4:HA:69:LYS:NZ | 2.16 | 0.78 |
| 5:K:353:HIS:HB2 | 7:BA:478:ASP:HB3 | 1.66 | 0.78 |
| 7:O:183:ALA:H | 7:O:189:GLY:HA3 | 1.49 | 0.78 |
| 13:YA:172[D]:PRO:HB3 | 13:YA:336[D]:LEU:HD22 | 1.65 | 0.78 |
| 13:YB:284[B]:MET:HE3 | 13:YC:363[B]:PRO:HB2 | 1.63 | 0.78 |
| 1:B:472:ASP:O | 1:B:473:HIS:ND1 | 2.15 | 0.78 |
| 10:BE:214:ARG:HH12 | 12:BG:246:ARG:HH12 | 1.31 | 0.78 |
| 5:CG:90:ASN:ND2 | 5:CH:49:TRP:O | 2.16 | 0.78 |
| 7:DC:78:PRO:HB3 | 7:DD:66:VAL:HA | 1.65 | 0.78 |
| 2:GF:548:ILE:HG12 | 2:GF:554:ASP:HB3 | 1.65 | 0.78 |
| 2:GF:782:VAL:HG21 | 2:GF:859:ARG:HB3 | 1.65 | 0.78 |
| 7:HJ:151:LEU:HB2 | 7:HJ:168:LEU:HD13 | 1.63 | 0.78 |
| 7:P:162:PRO:O | 7:P:166:GLN:N | 2.14 | 0.78 |
| 13:YB:172[E]:PRO:HB3 | 13:YB:336[E]:LEU:HD22 | 1.64 | 0.78 |
| 13:YC:172[A]:PRO:HB3 | 13:YC:336[A]:LEU:HD22 | 1.65 | 0.78 |
| 5:AC:186:TYR:OH | 5:AC:191:ILE:HA | 1.84 | 0.78 |
| 7:AI:401:ARG:HB3 | 7:BA:399:PHE:CE1 | 2.19 | 0.78 |
| 7:AJ:99:ARG:HD3 | 7:AJ:111:ASN:HD21 | 1.48 | 0.78 |
| 1:BH:389:ARG:NH2 | 1:BH:410:SER:OG | 2.17 | 0.78 |
| 3:CA:202:ARG:HB3 | 3:CA:209:VAL:HG21 | 1.63 | 0.78 |
| 5:CF:186:TYR:OH | 5:CF:191:ILE:HA | 1.84 | 0.78 |
| 1:BI:174:ARG:O | 11:DI:145:GLN:NE2 | 2.16 | 0.78 |
| 12:DJ:163:ARG:HG2 | 12:DJ:238:THR:HG22 | 1.64 | 0.78 |
| 2:EC:304:VAL:HG13 | 2:EC:327:ARG:HH12 | 1.48 | 0.78 |
| 2:EC:981:GLN:HG2 | 2:EC:982:LEU:H | 1.48 | 0.78 |
| 10:GA:214:ARG:HH12 | 12:GC:246:ARG:HH12 | 1.32 | 0.78 |
| 2:GF:304:VAL:HG13 | 2:GF:327:ARG:HH12 | 1.48 | 0.78 |
| 2:GF:981:GLN:HG2 | 2:GF:982:LEU:H | 1.48 | 0.78 |
| 8:FI:56:ARG:HD3 | 8:IB:64:ARG:HD3 | 1.65 | 0.78 |
| 7:O:473:LYS:HD2 | 7:Q:473:LYS:HB3 | 1.66 | 0.78 |
| 13:YB:208[E]:LYS:O | 13:YB:209[E]:GLN:NE2 | 2.17 | 0.78 |
| 5:AD:359:GLU:HB3 | 5:AD:370:HIS:HB3 | 1.64 | 0.78 |
| 2:BJ:304:VAL:HG13 | 2:BJ:327:ARG:HH12 | 1.48 | 0.78 |
| 2:BJ:366:TYR:HB2 | 2:BJ:380:ILE:HD11 | 1.64 | 0.78 |
| 2:C:304:VAL:HG13 | 2:C:327:ARG:HH12 | 1.48 | 0.78 |
| 5:CF:507:ASP:OD1 | 5:CF:511:ASN:N | 2.15 | 0.78 |
| 7:DB:386:ASN:OD1 | 7:DB:389:ASN:N | 2.17 | 0.78 |
| 2:EC:548:ILE:HG12 | 2:EC:554:ASP:HB3 | 1.65 | 0.78 |
| 5:EI:186:TYR:OH | 5:EI:191:ILE:HA | 1.84 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:412:PRO:HG3 | 7:FF:457:LEU:HD21 | 1.66 | 0.78 |
| 1:GE:45:ASP:O | 1:GE:47:ASP:N | 2.16 | 0.78 |
| 1:GE:23:GLY:N | 11:IE:26:THR:OG1 | 2.14 | 0.78 |
| 1:X:389:ARG:NH2 | 1:X:410:SER:OG | 2.17 | 0.78 |
| 13:YA:208[A]:LYS:O | 13:YA:209[A]:GLN:NE2 | 2.17 | 0.78 |
| 13:YA:382[A]:SER:OG | 13:YA:423[A]:GLU:OE2 | 2.00 | 0.78 |
| 13:YB:76[F]:PRO:HG3 | 13:YB:96[F]:VAL:HB | 1.62 | 0.78 |
| 7:DB:24:ASN:ND2 | 7:DD:45:ASN:OD1 | 2.15 | 0.78 |
| 5:FA:196:ARG:CZ | 7:FF:5:THR:HG23 | 2.12 | 0.78 |
| 13:YB:284[D]:MET:HE3 | 13:YC:363[D]:PRO:HB2 | 1.65 | 0.78 |
| 13:YC:382[C]:SER:OG | 13:YC:423[C]:GLU:OE2 | 2.01 | 0.78 |
| 1:B:346:ASP:OD1 | 1:B:347:THR:N | 2.15 | 0.78 |
| 5:CF:90:ASN:ND2 | 5:CG:49:TRP:O | 2.16 | 0.78 |
| 1:GD:317:GLY:HA3 | 1:GD:355:SER:HB2 | 1.66 | 0.78 |
| 1:GE:208:ASN:HB3 | 1:GE:224:TYR:CZ | 2.19 | 0.78 |
| 2:GF:206:GLN:N | 2:GF:206:GLN:OE1 | 2.15 | 0.78 |
| 6:HE:70:ILE:HG12 | 6:HF:73:ASN:HA | 1.66 | 0.78 |
| 5:I:90:ASN:ND2 | 5:J:49:TRP:O | 2.16 | 0.78 |
| 7:P:78:PRO:HB3 | 7:Q:66:VAL:HA | 1.66 | 0.78 |
| 10:U:214:ARG:HH12 | 12:W:246:ARG:HH12 | 1.31 | 0.78 |
| 1:X:317:GLY:HA3 | 1:X:355:SER:HB2 | 1.66 | 0.78 |
| 13:YA:8[A]:LEU:HD21 | 13:YB:10[A]:TRP:HB3 | 1.66 | 0.78 |
| 13:YB:172[C]:PRO:HB3 | 13:YB:336[C]:LEU:HD22 | 1.65 | 0.78 |
| 13:YC:172[B]:PRO:HB3 | 13:YC:336[B]:LEU:HD22 | 1.64 | 0.78 |
| 13:YC:44[B]:VAL:HG11 | 14:YE:272[B]:GLU:HB3 | 1.64 | 0.78 |
| 13:YB:554[C]:MET:HE2 | 13:YC:550[C]:TRP:CD1 | 2.19 | 0.78 |
| 7:AI:183:ALA:H | 7:AI:189:GLY:HA3 | 1.49 | 0.78 |
| 1:BH:99:LEU:HG | 1:BH:211:ARG:NH1 | 1.99 | 0.78 |
| 2:C:366:TYR:HB2 | 2:C:380:ILE:HD11 | 1.64 | 0.78 |
| 5:CH:339:GLU:HB2 | 6:CI:171:TYR:HB2 | 1.66 | 0.78 |
| 1:GE:555:ILE:HB | 1:GE:592:ILE:HD11 | 1.63 | 0.78 |
| 7:Q:117:THR:HG23 | 7:Q:120:LYS:H | 1.49 | 0.78 |
| 7:O:401:ARG:HB3 | 7:Q:399:PHE:CE1 | 2.19 | 0.78 |
| 1:X:99:LEU:HG | 1:X:211:ARG:NH1 | 1.99 | 0.78 |
| 1:Y:536:TYR:OH | 1:Y:562:ASP:OD2 | 2.01 | 0.78 |
| 13:YA:8[E]:LEU:HD21 | 13:YB:10[E]:TRP:HB3 | 1.66 | 0.78 |
| 13:YC:574[D]:ILE:O | 15:ZA:97[D]:LYS:N | 2.17 | 0.78 |
| 2:Z:124:GLN:O | 2:Z:128:THR:OG1 | 2.02 | 0.78 |
| 2:Z:366:TYR:HB2 | 2:Z:380:ILE:HD11 | 1.64 | 0.78 |
| 10:DH:214:ARG:HH12 | 12:DJ:246:ARG:HH12 | 1.31 | 0.78 |
| 1:EA:317:GLY:HA3 | 1:EA:355:SER:HB2 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:EF:103:LEU:HD21 | 4:EH:113:ASN:HD22 | 1.47 | 0.78 |
| 5:EJ:33:LEU:HA | 5:FA:43:PRO:HG3 | 1.65 | 0.78 |
| 5:EJ:188:VAL:HG11 | 5:FA:129:ARG:HE | 1.47 | 0.78 |
| 5:HC:359:GLU:HB3 | 5:HC:370:HIS:HB3 | 1.64 | 0.78 |
| 7:Q:101:SER:O | 7:Q:120:LYS:NZ | 2.16 | 0.78 |
| 2:Z:548:ILE:HG12 | 2:Z:554:ASP:HB3 | 1.65 | 0.78 |
| 7:AJ:78:PRO:HB3 | 7:BA:66:VAL:HA | 1.65 | 0.77 |
| 1:B:311:VAL:HG11 | 9:IC:20:ASN:HA | 1.65 | 0.77 |
| 5:CG:33:LEU:HA | 5:CH:43:PRO:HG3 | 1.63 | 0.77 |
| 7:HI:162:PRO:O | 7:HI:166:GLN:N | 2.14 | 0.77 |
| 13:YA:172[A]:PRO:HB3 | 13:YA:336[A]:LEU:HD22 | 1.65 | 0.77 |
| 13:YA:208[B]:LYS:O | 13:YA:209[B]:GLN:NE2 | 2.17 | 0.77 |
| 13:YB:172[D]:PRO:HB3 | 13:YB:336[D]:LEU:HD22 | 1.65 | 0.77 |
| 2:Z:782:VAL:HG21 | 2:Z:859:ARG:HB3 | 1.65 | 0.77 |
| 1:A:317:GLY:HA3 | 1:A:355:SER:HB2 | 1.66 | 0.77 |
| 1:A:389:ARG:NH2 | 1:A:410:SER:OG | 2.17 | 0.77 |
| 5:AD:318:GLN:NE2 | 6:AF:4:LEU:O | 2.17 | 0.77 |
| 1:BH:317:GLY:HA3 | 1:BH:355:SER:HB2 | 1.66 | 0.77 |
| 3:E:175:ASP:O | 3:E:189:GLU:HA | 1.84 | 0.77 |
| 1:EA:492:TYR:HA | 1:EA:606:ILE:HD12 | 1.65 | 0.77 |
| 1:GD:374:ILE:HB | 1:GD:408:ILE:HG12 | 1.64 | 0.77 |
| 6:HE:65:LYS:O | 6:HE:217:ARG:NH1 | 2.18 | 0.77 |
| 5:I:507:ASP:OD1 | 5:I:511:ASN:N | 2.15 | 0.77 |
| 5:K:260:ARG:O | 5:K:261:ARG:NH1 | 2.16 | 0.77 |
| 1:X:492:TYR:HA | 1:X:606:ILE:HD12 | 1.65 | 0.77 |
| 13:YC:172[C]:PRO:HB3 | 13:YC:336[C]:LEU:HD22 | 1.65 | 0.77 |
| 13:YC:208[E]:LYS:O | 13:YC:209[E]:GLN:NE2 | 2.17 | 0.77 |
| 13:YC:208[C]:LYS:O | 13:YC:209[C]:GLN:NE2 | 2.18 | 0.77 |
| 2:Z:420:THR:HG21 | 2:Z:423:GLU:HB2 | 1.67 | 0.77 |
| 5:AD:339:GLU:HB2 | 6:AH:171:TYR:HB2 | 1.66 | 0.77 |
| 2:BJ:548:ILE:HG12 | 2:BJ:554:ASP:HB3 | 1.65 | 0.77 |
| 6:CJ:65:LYS:O | 6:CJ:217:ARG:NH1 | 2.17 | 0.77 |
| 5:J:33:LEU:HA | 5:K:43:PRO:HG3 | 1.64 | 0.77 |
| 6:L:65:LYS:O | 6:L:217:ARG:NH1 | 2.18 | 0.77 |
| 13:YC:208[D]:LYS:O | 13:YC:209[D]:GLN:NE2 | 2.17 | 0.77 |
| 13:YC:574[C]:ILE:O | 15:ZA:97[C]:LYS:N | 2.17 | 0.77 |
| 5:AC:507:ASP:OD1 | 5:AC:511:ASN:N | 2.15 | 0.77 |
| 5:AE:260:ARG:O | 5:AE:261:ARG:NH1 | 2.16 | 0.77 |
| 7:BA:117:THR:HG23 | 7:BA:120:LYS:H | 1.49 | 0.77 |
| 5:CG:359:GLU:N | 5:CG:370:HIS:O | 2.17 | 0.77 |
| 7:DD:117:THR:HG23 | 7:DD:120:LYS:H | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:DG:20:ASN:HA | 1:EB:311:VAL:HG11 | 1.64 | 0.77 |
| 2:EC:782:VAL:HG21 | 2:EC:859:ARG:HB3 | 1.65 | 0.77 |
| 7:FG:117:THR:HG23 | 7:FG:120:LYS:H | 1.49 | 0.77 |
| 1:GD:99:LEU:HG | 1:GD:211:ARG:NH1 | 1.99 | 0.77 |
| 5:I:186:TYR:OH | 5:I:191:ILE:HA | 1.84 | 0.77 |
| 9:T:66:THR:H | 9:T:69:THR:HB | 1.49 | 0.77 |
| 13:YA:208[E]:LYS:O | 13:YA:209[E]:GLN:NE2 | 2.17 | 0.77 |
| 13:YA:172[F]:PRO:HB3 | 13:YA:336[F]:LEU:HD22 | 1.65 | 0.77 |
| 13:YC:57[B]:VAL:HG11 | 13:YC:76[B]:PRO:HD3 | 1.66 | 0.77 |
| 6:AG:65:LYS:O | 6:AG:217:ARG:NH1 | 2.18 | 0.77 |
| 2:BJ:782:VAL:HG21 | 2:BJ:859:ARG:HB3 | 1.65 | 0.77 |
| 2:C:168:ILE:HG23 | 2:C:169:GLY:H | 1.50 | 0.77 |
| 2:C:782:VAL:HG21 | 2:C:859:ARG:HB3 | 1.65 | 0.77 |
| 1:EA:389:ARG:NH2 | 1:EA:410:SER:OG | 2.17 | 0.77 |
| 1:EB:123:ILE:HD11 | 1:EB:295:ILE:HD11 | 1.66 | 0.77 |
| 2:EC:143:MET:HB2 | 2:EC:588:TYR:HD2 | 1.50 | 0.77 |
| 5:EJ:359:GLU:N | 5:EJ:370:HIS:O | 2.17 | 0.77 |
| 6:FD:65:LYS:O | 6:FD:217:ARG:NH1 | 2.18 | 0.77 |
| 7:FE:183:ALA:H | 7:FE:189:GLY:HA3 | 1.49 | 0.77 |
| 7:FE:386:ASN:OD1 | 7:FE:389:ASN:N | 2.17 | 0.77 |
| 5:HC:33:LEU:HA | 5:HD:43:PRO:HG3 | 1.65 | 0.77 |
| 5:I:326:MET:HG3 | 5:I:327:PRO:HD3 | 1.65 | 0.77 |
| 5:J:359:GLU:N | 5:J:370:HIS:O | 2.17 | 0.77 |
| 7:O:399:PHE:CE1 | 7:P:401:ARG:HB3 | 2.19 | 0.77 |
| 12:W:168:ALA:H | 12:IF:211:HIS:CE1 | 2.02 | 0.77 |
| 1:X:145:PHE:HB3 | 1:X:169:GLN:HA | 1.67 | 0.77 |
| 1:Y:45:ASP:O | 1:Y:47:ASP:N | 2.16 | 0.77 |
| 13:YB:208[A]:LYS:O | 13:YB:209[A]:GLN:NE2 | 2.17 | 0.77 |
| 7:AJ:476:ASP:O | 7:AJ:479:ASN:ND2 | 2.18 | 0.77 |
| 2:BJ:143:MET:HB2 | 2:BJ:588:TYR:HD2 | 1.50 | 0.77 |
| 5:CF:326:MET:HG3 | 5:CF:327:PRO:HD3 | 1.65 | 0.77 |
| 7:FE:473:LYS:HD2 | 7:FG:473:LYS:HB3 | 1.67 | 0.77 |
| 12:DJ:142:ASN:ND2 | 10:GA:210:ASP:O | 2.16 | 0.77 |
| 1:GE:123:ILE:HD11 | 1:GE:295:ILE:HD11 | 1.66 | 0.77 |
| 5:HB:186:TYR:OH | 5:HB:191:ILE:HA | 1.84 | 0.77 |
| 7:HH:401:ARG:HB3 | 7:HJ:399:PHE:CE1 | 2.19 | 0.77 |
| 7:HJ:117:THR:HG23 | 7:HJ:120:LYS:H | 1.49 | 0.77 |
| 1:X:210:THR:HG21 | 1:X:226:MET:HG2 | 1.67 | 0.77 |
| 13:YB:284[F]:MET:HE3 | 13:YC:363[F]:PRO:HB2 | 1.65 | 0.77 |
| 14:YD:174[C]:ARG:NH1 | 14:YD:188[C]:VAL:O | 2.18 | 0.77 |
| 14:YD:174[F]:ARG:NH1 | 14:YD:188[F]:VAL:O | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:174[A]:ARG:NH1 | 14:YE:188[A]:VAL:O | 2.18 | 0.77 |
| 14:YF:174[E]:ARG:NH1 | 14:YF:188[E]:VAL:O | 2.18 | 0.77 |
| 1:A:145:PHE:HB3 | 1:A:169:GLN:HA | 1.67 | 0.77 |
| 5:AC:90:ASN:ND2 | 5:AD:49:TRP:O | 2.16 | 0.77 |
| 5:AE:103:ASN:N | 5:AE:127:ASN:O | 2.14 | 0.77 |
| 6:AF:65:LYS:O | 6:AF:217:ARG:NH1 | 2.18 | 0.77 |
| 1:BI:123:ILE:HD11 | 1:BI:295:ILE:HD11 | 1.66 | 0.77 |
| 2:BJ:921:TRP:HE1 | 5:CG:19:LEU:HA | 1.47 | 0.77 |
| 2:C:124:GLN:O | 2:C:128:THR:OG1 | 2.02 | 0.77 |
| 6:CI:87:TYR:HB2 | 6:CI:181:GLU:HB2 | 1.67 | 0.77 |
| 7:DB:401:ARG:HB3 | 7:DD:399:PHE:CE1 | 2.20 | 0.77 |
| 1:EA:145:PHE:HB3 | 1:EA:169:GLN:HA | 1.67 | 0.77 |
| 1:EA:99:LEU:HG | 1:EA:211:ARG:NH1 | 1.99 | 0.77 |
| 6:HG:87:TYR:HB2 | 6:HG:181:GLU:HB2 | 1.67 | 0.77 |
| 5:I:339:GLU:HG2 | 6:M:173:THR:HB | 1.66 | 0.77 |
| 9:T:20:ASN:HA | 1:Y:311:VAL:HG11 | 1.64 | 0.77 |
| 13:YA:57[B]:VAL:HG11 | 13:YA:76[B]:PRO:HD3 | 1.66 | 0.77 |
| 13:YA:8[D]:LEU:HD21 | 13:YB:10[D]:TRP:HB3 | 1.66 | 0.77 |
| 13:YC:208[A]:LYS:O | 13:YC:209[A]:GLN:NE2 | 2.17 | 0.77 |
| 13:YC:208[B]:LYS:O | 13:YC:209[B]:GLN:NE2 | 2.17 | 0.77 |
| 14:YD:139[C]:ILE:O | 14:YD:143[C]:ARG:NH1 | 2.18 | 0.77 |
| 14:YE:139[C]:ILE:O | 14:YE:143[C]:ARG:NH1 | 2.18 | 0.77 |
| 2:Z:168:ILE:HG23 | 2:Z:169:GLY:H | 1.49 | 0.77 |
| 1:A:99:LEU:HG | 1:A:211:ARG:NH1 | 1.99 | 0.77 |
| 6:AF:87:TYR:HB2 | 6:AF:181:GLU:HB2 | 1.67 | 0.77 |
| 2:C:548:ILE:HG12 | 2:C:554:ASP:HB3 | 1.65 | 0.77 |
| 3:D:136:VAL:O | 3:D:150:LYS:NZ | 2.18 | 0.77 |
| 6:DA:65:LYS:O | 6:DA:217:ARG:NH1 | 2.18 | 0.77 |
| 6:DA:87:TYR:HB2 | 6:DA:181:GLU:HB2 | 1.67 | 0.77 |
| 1:EB:208:ASN:HB3 | 1:EB:224:TYR:CZ | 2.19 | 0.77 |
| 5:EI:507:ASP:OD1 | 5:EI:511:ASN:N | 2.15 | 0.77 |
| 6:FC:65:LYS:O | 6:FC:217:ARG:NH1 | 2.18 | 0.77 |
| 2:GF:124:GLN:O | 2:GF:128:THR:OG1 | 2.02 | 0.77 |
| 5:HC:44:TYR:HD2 | 5:HC:48:ALA:HB2 | 1.50 | 0.77 |
| 5:J:359:GLU:HB3 | 5:J:370:HIS:HB3 | 1.64 | 0.77 |
| 6:L:13:ARG:HG2 | 6:L:14:LEU:H | 1.50 | 0.77 |
| 6:N:65:LYS:O | 6:N:217:ARG:NH1 | 2.18 | 0.77 |
| 7:O:24:ASN:ND2 | 7:Q:45:ASN:OD1 | 2.18 | 0.77 |
| 7:P:476:ASP:O | 7:P:479:ASN:ND2 | 2.18 | 0.77 |
| 13:YA:8[F]:LEU:HD21 | 13:YB:10[F]:TRP:HB3 | 1.67 | 0.77 |
| 13:YB:208[B]:LYS:O | 13:YB:209[B]:GLN:NE2 | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:208[F]:LYS:O | 13:YB:209[F]:GLN:NE2 | 2.18 | 0.77 |
| 14:YE:174[D]:ARG:NH1 | 14:YE:188[D]:VAL:O | 2.18 | 0.77 |
| 13:YC:44[A]:VAL:HG11 | 14:YE:272[A]:GLU:HB3 | 1.64 | 0.77 |
| 5:AC:264:ARG:HB3 | 5:AE:326:MET:HE1 | 1.65 | 0.77 |
| 5:AC:326:MET:HG3 | 5:AC:327:PRO:HD3 | 1.65 | 0.77 |
| 1:EB:45:ASP:O | 1:EB:47:ASP:N | 2.16 | 0.77 |
| 4:GI:103:LEU:HD21 | 4:HA:113:ASN:HD22 | 1.50 | 0.77 |
| 5:HC:188:VAL:HG11 | 5:HD:129:ARG:HE | 1.48 | 0.77 |
| 6:HF:65:LYS:O | 6:HF:217:ARG:NH1 | 2.18 | 0.77 |
| 6:HG:13:ARG:HG2 | 6:HG:14:LEU:H | 1.50 | 0.77 |
| 9:IC:66:THR:H | 9:IC:69:THR:HB | 1.49 | 0.77 |
| 6:N:87:TYR:HB2 | 6:N:181:GLU:HB2 | 1.67 | 0.77 |
| 7:O:386:ASN:OD1 | 7:O:389:ASN:N | 2.17 | 0.77 |
| 13:YA:8[B]:LEU:HD21 | 13:YB:10[B]:TRP:HB3 | 1.66 | 0.77 |
| 13:YB:554[D]:MET:HE2 | 13:YC:550[D]:TRP:CD1 | 2.20 | 0.77 |
| 14:YF:174[A]:ARG:NH1 | 14:YF:188[A]:VAL:O | 2.18 | 0.77 |
| 14:YF:174[B]:ARG:NH1 | 14:YF:188[B]:VAL:O | 2.18 | 0.77 |
| 6:AH:87:TYR:HB2 | 6:AH:181:GLU:HB2 | 1.67 | 0.77 |
| 1:BI:208:ASN:HB3 | 1:BI:224:TYR:CZ | 2.19 | 0.77 |
| 11:DI:186:ARG:HG3 | 11:DI:187:ILE:HG12 | 1.67 | 0.77 |
| 12:DJ:211:HIS:CE1 | 12:GC:168:ALA:H | 2.02 | 0.77 |
| 2:GF:928:GLU:HG3 | 2:GF:929:TYR:H | 1.50 | 0.77 |
| 13:YA:208[C]:LYS:O | 13:YA:209[C]:GLN:NE2 | 2.18 | 0.77 |
| 13:YB:554[E]:MET:HE2 | 13:YC:550[E]:TRP:CD1 | 2.20 | 0.77 |
| 14:YD:174[E]:ARG:NH1 | 14:YD:188[E]:VAL:O | 2.18 | 0.77 |
| 14:YE:174[C]:ARG:NH1 | 14:YE:188[C]:VAL:O | 2.18 | 0.77 |
| 6:AG:13:ARG:HG2 | 6:AG:14:LEU:H | 1.50 | 0.76 |
| 2:BJ:124:GLN:O | 2:BJ:128:THR:OG1 | 2.02 | 0.76 |
| 2:C:981:GLN:HG2 | 2:C:982:LEU:H | 1.48 | 0.76 |
| 6:CI:65:LYS:O | 6:CI:217:ARG:NH1 | 2.18 | 0.76 |
| 5:EI:326:MET:HG3 | 5:EI:327:PRO:HD3 | 1.65 | 0.76 |
| 7:HH:473:LYS:HD2 | 7:HJ:473:LYS:HB3 | 1.67 | 0.76 |
| 7:Q:365:GLY:HA2 | 7:HI:71:ASN:HB2 | 1.67 | 0.76 |
| 13:YA:208[D]:LYS:O | 13:YA:209[D]:GLN:NE2 | 2.17 | 0.76 |
| 13:YB:208[C]:LYS:O | 13:YB:209[C]:GLN:NE2 | 2.18 | 0.76 |
| 13:YB:208[D]:LYS:O | 13:YB:209[D]:GLN:NE2 | 2.17 | 0.76 |
| 13:YB:554[B]:MET:HE2 | 13:YC:550[B]:TRP:CD1 | 2.19 | 0.76 |
| 14:YE:174[F]:ARG:NH1 | 14:YE:188[F]:VAL:O | 2.18 | 0.76 |
| 6:AH:13:ARG:HG2 | 6:AH:14:LEU:H | 1.50 | 0.76 |
| 1:B:208:ASN:HB3 | 1:B:224:TYR:CZ | 2.19 | 0.76 |
| 7:DB:183:ALA:H | 7:DB:189:GLY:HA3 | 1.49 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:90:ASN:ND2 | 5:EJ:49:TRP:O | 2.17 | 0.76 |
| 2:GF:160:VAL:HA | 2:GF:163:ILE:HD12 | 1.67 | 0.76 |
| 3:GG:136:VAL:O | 3:GG:150:LYS:NZ | 2.18 | 0.76 |
| 3:GG:149:ASP:OD2 | 3:GG:152:GLU:N | 2.17 | 0.76 |
| 5:HB:90:ASN:ND2 | 5:HC:49:TRP:O | 2.16 | 0.76 |
| 7:HH:386:ASN:OD1 | 7:HH:389:ASN:N | 2.17 | 0.76 |
| 6:L:28:ASP:OD2 | 6:M:60:HIS:NE2 | 2.19 | 0.76 |
| 13:YB:284[C]:MET:HE3 | 13:YC:363[C]:PRO:HB2 | 1.64 | 0.76 |
| 13:YB:284[E]:MET:HE3 | 13:YC:363[E]:PRO:HB2 | 1.68 | 0.76 |
| 14:YE:139[A]:ILE:O | 14:YE:143[A]:ARG:NH1 | 2.18 | 0.76 |
| 14:YF:174[D]:ARG:NH1 | 14:YF:188[D]:VAL:O | 2.18 | 0.76 |
| 13:YC:574[B]:ILE:O | 15:ZA:97[B]:LYS:N | 2.17 | 0.76 |
| 13:YC:574[E]:ILE:O | 15:ZA:97[E]:LYS:N | 2.17 | 0.76 |
| 5:AD:359:GLU:N | 5:AD:370:HIS:O | 2.17 | 0.76 |
| 5:J:412:PRO:HG3 | 7:AJ:457:LEU:HD21 | 1.65 | 0.76 |
| 2:EC:928:GLU:HG3 | 2:EC:929:TYR:H | 1.50 | 0.76 |
| 3:EE:175:ASP:O | 3:EE:189:GLU:HA | 1.84 | 0.76 |
| 6:FC:13:ARG:HG2 | 6:FC:14:LEU:H | 1.50 | 0.76 |
| 6:HF:13:ARG:HG2 | 6:HF:14:LEU:H | 1.50 | 0.76 |
| 7:HH:24:ASN:ND2 | 7:HJ:45:ASN:OD1 | 2.18 | 0.76 |
| 6:M:87:TYR:HB2 | 6:M:181:GLU:HB2 | 1.67 | 0.76 |
| 13:YA:208[F]:LYS:O | 13:YA:209[F]:GLN:NE2 | 2.18 | 0.76 |
| 13:YB:284[A]:MET:HE3 | 13:YC:363[A]:PRO:HB2 | 1.65 | 0.76 |
| 14:YD:174[D]:ARG:NH1 | 14:YD:188[D]:VAL:O | 2.18 | 0.76 |
| 14:YE:253[B]:ILE:HG12 | 14:YE:275[B]:ILE:HB | 1.68 | 0.76 |
| 14:YF:139[A]:ILE:O | 14:YF:143[A]:ARG:NH1 | 2.18 | 0.76 |
| 5:AD:44:TYR:HD2 | 5:AD:48:ALA:HB2 | 1.50 | 0.76 |
| 2:C:160:VAL:HA | 2:C:163:ILE:HD12 | 1.67 | 0.76 |
| 6:FB:87:TYR:HB2 | 6:FB:181:GLU:HB2 | 1.67 | 0.76 |
| 5:HC:359:GLU:N | 5:HC:370:HIS:O | 2.17 | 0.76 |
| 7:HH:183:ALA:H | 7:HH:189:GLY:HA3 | 1.49 | 0.76 |
| 6:M:65:LYS:O | 6:M:217:ARG:NH1 | 2.18 | 0.76 |
| 13:YC:208[F]:LYS:O | 13:YC:209[F]:GLN:NE2 | 2.17 | 0.76 |
| 14:YD:174[B]:ARG:NH1 | 14:YD:188[B]:VAL:O | 2.18 | 0.76 |
| 14:YE:174[B]:ARG:NH1 | 14:YE:188[B]:VAL:O | 2.18 | 0.76 |
| 14:YF:139[D]:ILE:O | 14:YF:143[D]:ARG:NH1 | 2.18 | 0.76 |
| 14:YF:174[F]:ARG:NH1 | 14:YF:188[F]:VAL:O | 2.18 | 0.76 |
| 14:YF:253[F]:ILE:HG12 | 14:YF:275[F]:ILE:HB | 1.68 | 0.76 |
| 5:AE:180:VAL:HG11 | 5:AE:186:TYR:HB2 | 1.68 | 0.76 |
| 7:AI:24:ASN:ND2 | 7:BA:45:ASN:OD1 | 2.18 | 0.76 |
| 11:BF:186:ARG:HG3 | 11:BF:187:ILE:HG12 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DC:476:ASP:O | 7:DC:479:ASN:ND2 | 2.18 | 0.76 |
| 6:FD:87:TYR:HB2 | 6:FD:181:GLU:HB2 | 1.67 | 0.76 |
| 6:HG:65:LYS:O | 6:HG:217:ARG:NH1 | 2.17 | 0.76 |
| 7:HH:399:PHE:CE1 | 7:HI:401:ARG:HB3 | 2.21 | 0.76 |
| 13:YB:397[C]:SER:OG | 13:YC:405[C]:ASP:OD1 | 2.04 | 0.76 |
| 14:YD:139[B]:ILE:O | 14:YD:143[B]:ARG:NH1 | 2.18 | 0.76 |
| 14:YE:30[A]:GLU:OE2 | 14:YE:32[A]:ALA:N | 2.19 | 0.76 |
| 14:YF:139[C]:ILE:O | 14:YF:143[C]:ARG:NH1 | 2.18 | 0.76 |
| 14:YF:139[E]:ILE:O | 14:YF:143[E]:ARG:NH1 | 2.19 | 0.76 |
| 14:YF:30[E]:GLU:OE2 | 14:YF:32[E]:ALA:N | 2.19 | 0.76 |
| 13:YC:574[F]:ILE:O | 15:ZA:97[F]:LYS:N | 2.17 | 0.76 |
| 1:A:210:THR:HG21 | 1:A:226:MET:HG2 | 1.67 | 0.76 |
| 7:AI:473:LYS:HD2 | 7:BA:473:LYS:HB3 | 1.67 | 0.76 |
| 5:CH:180:VAL:HG11 | 5:CH:186:TYR:HB2 | 1.68 | 0.76 |
| 2:GF:143:MET:HB2 | 2:GF:588:TYR:HD2 | 1.50 | 0.76 |
| 6:HF:87:TYR:HB2 | 6:HF:181:GLU:HB2 | 1.67 | 0.76 |
| 1:Y:208:ASN:HB3 | 1:Y:224:TYR:CZ | 2.19 | 0.76 |
| 14:YD:139[E]:ILE:O | 14:YD:143[E]:ARG:NH1 | 2.19 | 0.76 |
| 14:YD:30[C]:GLU:OE2 | 14:YD:32[C]:ALA:N | 2.19 | 0.76 |
| 14:YE:253[A]:ILE:HG12 | 14:YE:275[A]:ILE:HB | 1.68 | 0.76 |
| 2:Z:438:GLY:O | 2:Z:439:LYS:HG2 | 1.86 | 0.76 |
| 5:K:363:ASN:HB2 | 7:BA:473:LYS:HG2 | 1.68 | 0.76 |
| 3:CA:136:VAL:O | 3:CA:150:LYS:NZ | 2.18 | 0.76 |
| 2:EC:168:ILE:HG23 | 2:EC:169:GLY:H | 1.50 | 0.76 |
| 2:EC:420:THR:HG21 | 2:EC:423:GLU:HB2 | 1.66 | 0.76 |
| 3:ED:136:VAL:O | 3:ED:150:LYS:NZ | 2.18 | 0.76 |
| 5:EJ:79:ILE:HD12 | 5:EJ:81:LEU:HD11 | 1.66 | 0.76 |
| 5:FA:318:GLN:NE2 | 6:FC:4:LEU:O | 2.18 | 0.76 |
| 3:GH:175:ASP:O | 3:GH:189:GLU:HA | 1.85 | 0.76 |
| 7:HI:476:ASP:O | 7:HI:479:ASN:ND2 | 2.18 | 0.76 |
| 5:J:44:TYR:HD2 | 5:J:48:ALA:HB2 | 1.50 | 0.76 |
| 5:J:79:ILE:HD12 | 5:J:81:LEU:HD11 | 1.66 | 0.76 |
| 6:M:13:ARG:HG2 | 6:M:14:LEU:H | 1.50 | 0.76 |
| 13:YB:61[F]:ILE:HB | 13:YC:75[F]:GLY:HA2 | 1.68 | 0.76 |
| 14:YD:253[D]:ILE:HG12 | 14:YD:275[D]:ILE:HB | 1.68 | 0.76 |
| 14:YF:139[B]:ILE:O | 14:YF:143[B]:ARG:NH1 | 2.18 | 0.76 |
| 5:CG:326:MET:HG3 | 5:CG:327:PRO:HD3 | 1.68 | 0.76 |
| 2:EC:124:GLN:O | 2:EC:128:THR:OG1 | 2.02 | 0.76 |
| 1:GD:145:PHE:HB3 | 1:GD:169:GLN:HA | 1.67 | 0.76 |
| 5:HD:180:VAL:HG11 | 5:HD:186:TYR:HB2 | 1.68 | 0.76 |
| 5:K:180:VAL:HG11 | 5:K:186:TYR:HB2 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:339:GLU:HB2 | 6:L:171:TYR:HB2 | 1.67 | 0.76 |
| 13:YB:397[D]:SER:OG | 13:YC:405[D]:ASP:OD1 | 2.04 | 0.76 |
| 13:YA:60[E]:PRO:HD3 | 13:YC:61[E]:ILE:HG23 | 1.66 | 0.76 |
| 14:YD:253[C]:ILE:HG12 | 14:YD:275[C]:ILE:HB | 1.68 | 0.76 |
| 14:YE:215[F]:GLU:OE1 | 14:YF:100[F]:LYS:NZ | 2.19 | 0.76 |
| 14:YF:253[E]:ILE:HG12 | 14:YF:275[E]:ILE:HB | 1.68 | 0.76 |
| 7:AI:170:ILE:O | 7:AI:174:ALA:N | 2.19 | 0.76 |
| 2:BJ:420:THR:HG21 | 2:BJ:423:GLU:HB2 | 1.67 | 0.76 |
| 2:C:69:PHE:CZ | 2:C:71:ASP:HB2 | 2.21 | 0.76 |
| 5:CG:44:TYR:HD2 | 5:CG:48:ALA:HB2 | 1.50 | 0.76 |
| 6:DA:13:ARG:HG2 | 6:DA:14:LEU:H | 1.50 | 0.76 |
| 9:DG:66:THR:H | 9:DG:69:THR:HB | 1.49 | 0.76 |
| 5:HB:326:MET:HG3 | 5:HB:327:PRO:HD3 | 1.65 | 0.76 |
| 6:N:13:ARG:HG2 | 6:N:14:LEU:H | 1.50 | 0.76 |
| 8:S:74:MET:HA | 8:S:152:THR:HG22 | 1.68 | 0.76 |
| 1:Y:455:PHE:HD1 | 1:Y:639:LEU:HD12 | 1.50 | 0.76 |
| 13:YB:57[B]:VAL:HG11 | 13:YB:76[B]:PRO:HD3 | 1.66 | 0.76 |
| 14:YD:139[A]:ILE:O | 14:YD:143[A]:ARG:NH1 | 2.19 | 0.76 |
| 14:YD:30[F]:GLU:OE2 | 14:YD:32[F]:ALA:N | 2.19 | 0.76 |
| 14:YE:139[D]:ILE:O | 14:YE:143[D]:ARG:NH1 | 2.18 | 0.76 |
| 13:YB:90[E]:TRP:NE1 | 14:YE:175[E]:GLU:OE1 | 2.19 | 0.76 |
| 14:YF:30[B]:GLU:OE2 | 14:YF:32[B]:ALA:N | 2.19 | 0.76 |
| 7:AI:24:ASN:ND2 | 7:BA:41:PRO:HA | 2.00 | 0.76 |
| 1:BH:290:ASP:OD1 | 1:BH:291:THR:N | 2.19 | 0.76 |
| 7:DB:170:ILE:O | 7:DB:174:ALA:N | 2.19 | 0.76 |
| 1:EA:290:ASP:OD1 | 1:EA:291:THR:N | 2.19 | 0.76 |
| 1:EB:536:TYR:OH | 1:EB:562:ASP:OD2 | 2.01 | 0.76 |
| 5:EI:285:LEU:HD11 | 5:EI:375:PHE:HB2 | 1.68 | 0.76 |
| 5:EJ:44:TYR:HD2 | 5:EJ:48:ALA:HB2 | 1.50 | 0.76 |
| 6:FB:65:LYS:O | 6:FB:217:ARG:NH1 | 2.18 | 0.76 |
| 7:FE:399:PHE:CE1 | 7:FF:401:ARG:HB3 | 2.21 | 0.76 |
| 11:GB:186:ARG:HG3 | 11:GB:187:ILE:HG12 | 1.68 | 0.76 |
| 1:GD:389:ARG:NH2 | 1:GD:410:SER:OG | 2.17 | 0.76 |
| 4:GJ:69:LYS:NZ | 4:HA:103:LEU:O | 2.17 | 0.76 |
| 6:HE:87:TYR:HB2 | 6:HE:181:GLU:HB2 | 1.67 | 0.76 |
| 7:P:27:PRO:HA | 7:P:29:ILE:HD11 | 1.68 | 0.76 |
| 13:YA:8[C]:LEU:HD21 | 13:YB:10[C]:TRP:HB3 | 1.67 | 0.76 |
| 14:YE:139[F]:ILE:O | 14:YE:143[F]:ARG:NH1 | 2.19 | 0.76 |
| 6:AH:65:LYS:O | 6:AH:217:ARG:NH1 | 2.18 | 0.75 |
| 1:BH:145:PHE:HB3 | 1:BH:169:GLN:HA | 1.67 | 0.75 |
| 2:BJ:438:GLY:O | 2:BJ:439:LYS:HG2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:79:ILE:HD12 | 5:CG:81:LEU:HD11 | 1.66 | 0.75 |
| 4:EG:113:ASN:HD22 | 4:EH:103:LEU:HD21 | 1.52 | 0.75 |
| 5:FA:180:VAL:HG11 | 5:FA:186:TYR:HB2 | 1.68 | 0.75 |
| 6:FD:13:ARG:HG2 | 6:FD:14:LEU:H | 1.50 | 0.75 |
| 7:FE:24:ASN:ND2 | 7:FG:41:PRO:HA | 2.00 | 0.75 |
| 7:FF:57:ILE:HG22 | 7:FG:55:LYS:HB3 | 1.66 | 0.75 |
| 2:EC:474:GLU:HB3 | 3:GH:155:LYS:HE2 | 1.67 | 0.75 |
| 4:GJ:113:ASN:HD22 | 4:HA:103:LEU:HD21 | 1.51 | 0.75 |
| 13:YC:184[F]:GLU:HG2 | 13:YC:203[F]:GLY:HA3 | 1.69 | 0.75 |
| 13:YB:397[B]:SER:OG | 13:YC:405[B]:ASP:OD1 | 2.04 | 0.75 |
| 14:YD:41[C]:ARG:NH2 | 14:YD:341[C]:GLU:OE2 | 2.19 | 0.75 |
| 14:YE:41[D]:ARG:NH2 | 14:YE:341[D]:GLU:OE2 | 2.19 | 0.75 |
| 14:YF:253[A]:ILE:HG12 | 14:YF:275[A]:ILE:HB | 1.68 | 0.75 |
| 14:YF:30[F]:GLU:OE2 | 14:YF:32[F]:ALA:N | 2.19 | 0.75 |
| 5:AD:79:ILE:HD12 | 5:AD:81:LEU:HD11 | 1.66 | 0.75 |
| 1:B:494:THR:HG21 | 1:B:603:TYR:HA | 1.69 | 0.75 |
| 1:BH:210:THR:HG21 | 1:BH:226:MET:HG2 | 1.67 | 0.75 |
| 2:BJ:168:ILE:HG23 | 2:BJ:169:GLY:H | 1.50 | 0.75 |
| 7:FF:291:ARG:NH2 | 7:FG:269:ALA:O | 2.18 | 0.75 |
| 9:FJ:66:THR:H | 9:FJ:69:THR:HB | 1.49 | 0.75 |
| 2:GF:39:ALA:HB3 | 2:GF:79:ILE:HB | 1.69 | 0.75 |
| 6:HE:13:ARG:HG2 | 6:HE:14:LEU:H | 1.50 | 0.75 |
| 8:IA:74:MET:HA | 8:IA:152:THR:HG22 | 1.68 | 0.75 |
| 1:Y:123:ILE:HD11 | 1:Y:295:ILE:HD11 | 1.66 | 0.75 |
| 14:YE:139[E]:ILE:O | 14:YE:143[E]:ARG:NH1 | 2.19 | 0.75 |
| 14:YE:174[E]:ARG:NH1 | 14:YE:188[E]:VAL:O | 2.18 | 0.75 |
| 14:YE:253[C]:ILE:HG12 | 14:YE:275[C]:ILE:HB | 1.68 | 0.75 |
| 14:YE:30[B]:GLU:OE2 | 14:YE:32[B]:ALA:N | 2.19 | 0.75 |
| 14:YE:30[D]:GLU:OE2 | 14:YE:32[D]:ALA:N | 2.19 | 0.75 |
| 14:YF:41[B]:ARG:NH2 | 14:YF:341[B]:GLU:OE2 | 2.19 | 0.75 |
| 14:YF:41[E]:ARG:NH2 | 14:YF:341[E]:GLU:OE2 | 2.19 | 0.75 |
| 6:AF:70:ILE:HG12 | 6:AG:73:ASN:HA | 1.69 | 0.75 |
| 1:B:123:ILE:HD11 | 1:B:295:ILE:HD11 | 1.66 | 0.75 |
| 9:BD:66:THR:H | 9:BD:69:THR:HB | 1.49 | 0.75 |
| 2:C:420:THR:HG21 | 2:C:423:GLU:HB2 | 1.67 | 0.75 |
| 2:C:438:GLY:O | 2:C:439:LYS:HG2 | 1.86 | 0.75 |
| 7:DB:212:PRO:HB2 | 7:DC:203:THR:HG22 | 1.69 | 0.75 |
| 2:EC:160:VAL:HA | 2:EC:163:ILE:HD12 | 1.67 | 0.75 |
| 2:EC:39:ALA:HB3 | 2:EC:79:ILE:HB | 1.69 | 0.75 |
| 6:CI:77:VAL:HG23 | 7:FF:167:GLN:HE21 | 1.51 | 0.75 |
| 7:FF:476:ASP:O | 7:FF:479:ASN:ND2 | 2.18 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:79:ILE:HD12 | 5:HC:81:LEU:HD11 | 1.66 | 0.75 |
| 7:HH:132:ARG:NH1 | 7:HJ:126:ASN:OD1 | 2.19 | 0.75 |
| 13:YB:90[D]:TRP:NE1 | 14:YE:175[D]:GLU:OE1 | 2.19 | 0.75 |
| 13:YB:397[E]:SER:OG | 13:YC:405[E]:ASP:OD1 | 2.04 | 0.75 |
| 14:YD:139[D]:ILE:O | 14:YD:143[D]:ARG:NH1 | 2.18 | 0.75 |
| 14:YD:139[F]:ILE:O | 14:YD:143[F]:ARG:NH1 | 2.19 | 0.75 |
| 14:YD:30[E]:GLU:OE2 | 14:YD:32[E]:ALA:N | 2.19 | 0.75 |
| 14:YD:41[D]:ARG:NH2 | 14:YD:341[D]:GLU:OE2 | 2.19 | 0.75 |
| 14:YE:139[B]:ILE:O | 14:YE:143[B]:ARG:NH1 | 2.18 | 0.75 |
| 14:YE:30[E]:GLU:OE2 | 14:YE:32[E]:ALA:N | 2.19 | 0.75 |
| 14:YF:30[A]:GLU:OE2 | 14:YF:32[A]:ALA:N | 2.19 | 0.75 |
| 1:A:290:ASP:OD1 | 1:A:291:THR:N | 2.19 | 0.75 |
| 5:AE:34:TYR:O | 5:AE:38:GLY:N | 2.20 | 0.75 |
| 2:C:39:ALA:HB3 | 2:C:79:ILE:HB | 1.69 | 0.75 |
| 5:CF:285:LEU:HD11 | 5:CF:375:PHE:HB2 | 1.68 | 0.75 |
| 1:EB:455:PHE:HD1 | 1:EB:639:LEU:HD12 | 1.50 | 0.75 |
| 2:GF:420:THR:HG21 | 2:GF:423:GLU:HB2 | 1.67 | 0.75 |
| 5:HB:299:ILE:O | 5:HB:301:GLY:N | 2.20 | 0.75 |
| 1:GE:174:ARG:O | 11:IE:145:GLN:NE2 | 2.19 | 0.75 |
| 6:L:87:TYR:HB2 | 6:L:181:GLU:HB2 | 1.67 | 0.75 |
| 6:L:70:ILE:HG12 | 6:M:73:ASN:HA | 1.69 | 0.75 |
| 14:YD:174[A]:ARG:NH1 | 14:YD:188[A]:VAL:O | 2.18 | 0.75 |
| 14:YD:253[E]:ILE:HG12 | 14:YD:275[E]:ILE:HB | 1.68 | 0.75 |
| 14:YD:30[D]:GLU:OE2 | 14:YD:32[D]:ALA:N | 2.19 | 0.75 |
| 14:YD:30[A]:GLU:OE2 | 14:YD:32[A]:ALA:N | 2.19 | 0.75 |
| 14:YD:41[F]:ARG:NH2 | 14:YD:341[F]:GLU:OE2 | 2.19 | 0.75 |
| 14:YE:30[C]:GLU:OE2 | 14:YE:32[C]:ALA:N | 2.19 | 0.75 |
| 6:AF:13:ARG:HG2 | 6:AF:14:LEU:H | 1.50 | 0.75 |
| 1:BI:455:PHE:HD1 | 1:BI:639:LEU:HD12 | 1.50 | 0.75 |
| 5:CG:339:GLU:HB2 | 6:DA:171:TYR:HB2 | 1.68 | 0.75 |
| 1:EB:174:ARG:O | 11:GB:145:GLN:NE2 | 2.19 | 0.75 |
| 2:GF:933:ILE:HG12 | 2:GF:935:LYS:H | 1.52 | 0.75 |
| 5:HD:261:ARG:HB2 | 5:HD:383:ILE:HB | 1.68 | 0.75 |
| 1:Y:494:THR:HG21 | 1:Y:603:TYR:HA | 1.69 | 0.75 |
| 14:YD:253[F]:ILE:HG12 | 14:YD:275[F]:ILE:HB | 1.68 | 0.75 |
| 14:YE:41[E]:ARG:NH2 | 14:YE:341[E]:GLU:OE2 | 2.19 | 0.75 |
| 14:YF:253[B]:ILE:HG12 | 14:YF:275[B]:ILE:HB | 1.68 | 0.75 |
| 14:YF:30[C]:GLU:OE2 | 14:YF:32[C]:ALA:N | 2.19 | 0.75 |
| 14:YF:41[C]:ARG:NH2 | 14:YF:341[C]:GLU:OE2 | 2.19 | 0.75 |
| 1:BI:325:ILE:O | 1:BI:329:GLY:N | 2.15 | 0.75 |
| 3:CB:175:ASP:O | 3:CB:189:GLU:HA | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:399:PHE:CE1 | 7:DC:401:ARG:HB3 | 2.21 | 0.75 |
| 3:E:195:PRO:HD3 | 3:E:223:TRP:CD1 | 2.22 | 0.75 |
| 1:EA:210:THR:HG21 | 1:EA:226:MET:HG2 | 1.67 | 0.75 |
| 2:EC:933:ILE:HG12 | 2:EC:935:LYS:H | 1.52 | 0.75 |
| 3:EE:195:PRO:HD3 | 3:EE:223:TRP:CD1 | 2.22 | 0.75 |
| 5:EJ:326:MET:HG3 | 5:EJ:327:PRO:HD3 | 1.68 | 0.75 |
| 8:FH:74:MET:HA | 8:FH:152:THR:HG22 | 1.68 | 0.75 |
| 1:GD:210:THR:HG21 | 1:GD:226:MET:HG2 | 1.67 | 0.75 |
| 2:GF:168:ILE:HG23 | 2:GF:169:GLY:H | 1.50 | 0.75 |
| 5:HB:285:LEU:HD11 | 5:HB:375:PHE:HB2 | 1.68 | 0.75 |
| 11:IE:186:ARG:HG3 | 11:IE:187:ILE:HG12 | 1.67 | 0.75 |
| 5:J:339:GLU:HB2 | 6:N:171:TYR:HB2 | 1.68 | 0.75 |
| 1:X:290:ASP:OD1 | 1:X:291:THR:N | 2.19 | 0.75 |
| 1:Y:325:ILE:O | 1:Y:329:GLY:N | 2.15 | 0.75 |
| 13:YA:184[D]:GLU:HG2 | 13:YA:203[D]:GLY:HA3 | 1.69 | 0.75 |
| 13:YA:61[E]:ILE:HG21 | 13:YB:59[E]:GLN:HA | 1.67 | 0.75 |
| 14:YD:215[D]:GLU:OE1 | 14:YE:100[D]:LYS:NZ | 2.20 | 0.75 |
| 14:YE:253[F]:ILE:HG12 | 14:YE:275[F]:ILE:HB | 1.68 | 0.75 |
| 14:YE:41[A]:ARG:NH2 | 14:YE:341[A]:GLU:OE2 | 2.19 | 0.75 |
| 14:YE:41[B]:ARG:NH2 | 14:YE:341[B]:GLU:OE2 | 2.19 | 0.75 |
| 14:YF:174[C]:ARG:NH1 | 14:YF:188[C]:VAL:O | 2.18 | 0.75 |
| 2:Z:200:TYR:OH | 2:Z:292:GLU:OE1 | 2.04 | 0.75 |
| 2:Z:39:ALA:HB3 | 2:Z:79:ILE:HB | 1.69 | 0.75 |
| 2:Z:69:PHE:CZ | 2:Z:71:ASP:HB2 | 2.21 | 0.75 |
| 7:AI:132:ARG:NH1 | 7:BA:126:ASN:OD1 | 2.19 | 0.75 |
| 5:CF:321:ALA:HA | 5:CF:358:VAL:HB | 1.68 | 0.75 |
| 5:CH:34:TYR:O | 5:CH:38:GLY:N | 2.20 | 0.75 |
| 6:CI:28:ASP:OD2 | 6:CJ:60:HIS:NE2 | 2.18 | 0.75 |
| 6:CJ:13:ARG:HG2 | 6:CJ:14:LEU:H | 1.50 | 0.75 |
| 1:BI:23:GLY:N | 11:DI:26:THR:OG1 | 2.16 | 0.75 |
| 5:EI:321:ALA:HA | 5:EI:358:VAL:HB | 1.68 | 0.75 |
| 1:EB:23:GLY:N | 11:GB:26:THR:OG1 | 2.14 | 0.75 |
| 5:HC:84:GLY:O | 5:HC:86:VAL:N | 2.19 | 0.75 |
| 7:HH:13:SER:HB2 | 7:HI:18:PHE:HA | 1.68 | 0.75 |
| 11:IE:46:ARG:HD2 | 11:IE:173:ALA:HB2 | 1.69 | 0.75 |
| 13:YA:184[C]:GLU:HG2 | 13:YA:203[C]:GLY:HA3 | 1.69 | 0.75 |
| 13:YC:184[A]:GLU:HG2 | 13:YC:203[A]:GLY:HA3 | 1.69 | 0.75 |
| 14:YD:253[B]:ILE:HG12 | 14:YD:275[B]:ILE:HB | 1.68 | 0.75 |
| 14:YF:41[F]:ARG:NH2 | 14:YF:341[F]:GLU:OE2 | 2.19 | 0.75 |
| 2:Z:143:MET:HB2 | 2:Z:588:TYR:HD2 | 1.50 | 0.75 |
| 2:Z:928:GLU:HG3 | 2:Z:929:TYR:H | 1.50 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:261:ARG:HB2 | 5:AE:383:ILE:HB | 1.68 | 0.75 |
| 2:C:143:MET:HB2 | 2:C:588:TYR:HD2 | 1.50 | 0.75 |
| 7:FE:170:ILE:O | 7:FE:174:ALA:N | 2.19 | 0.75 |
| 1:GE:494:THR:HG21 | 1:GE:603:TYR:HA | 1.69 | 0.75 |
| 7:HI:191:VAL:O | 7:HJ:189:GLY:N | 2.20 | 0.75 |
| 7:HI:27:PRO:HA | 7:HI:29:ILE:HD11 | 1.68 | 0.75 |
| 5:J:326:MET:HG3 | 5:J:327:PRO:HD3 | 1.68 | 0.75 |
| 14:YD:30[B]:GLU:OE2 | 14:YD:32[B]:ALA:N | 2.19 | 0.75 |
| 14:YE:250[E]:ASN:HD21 | 14:YE:272[E]:GLU:HB2 | 1.52 | 0.75 |
| 14:YE:30[F]:GLU:OE2 | 14:YE:32[F]:ALA:N | 2.19 | 0.75 |
| 14:YF:139[F]:ILE:O | 14:YF:143[F]:ARG:NH1 | 2.19 | 0.75 |
| 2:Z:160:VAL:HA | 2:Z:163:ILE:HD12 | 1.67 | 0.75 |
| 2:BJ:160:VAL:HA | 2:BJ:163:ILE:HD12 | 1.67 | 0.75 |
| 2:BJ:933:ILE:HG12 | 2:BJ:935:LYS:H | 1.52 | 0.75 |
| 2:C:928:GLU:HG3 | 2:C:929:TYR:H | 1.50 | 0.75 |
| 5:CH:84:GLY:O | 5:CH:86:VAL:N | 2.20 | 0.75 |
| 2:EC:438:GLY:O | 2:EC:439:LYS:HG2 | 1.86 | 0.75 |
| 6:FB:13:ARG:HG2 | 6:FB:14:LEU:H | 1.50 | 0.75 |
| 7:O:170:ILE:O | 7:O:174:ALA:N | 2.19 | 0.75 |
| 13:YB:184[B]:GLU:HG2 | 13:YB:203[B]:GLY:HA3 | 1.69 | 0.75 |
| 13:YB:184[C]:GLU:HG2 | 13:YB:203[C]:GLY:HA3 | 1.69 | 0.75 |
| 14:YD:253[A]:ILE:HG12 | 14:YD:275[A]:ILE:HB | 1.68 | 0.75 |
| 14:YE:253[D]:ILE:HG12 | 14:YE:275[D]:ILE:HB | 1.68 | 0.75 |
| 14:YF:253[D]:ILE:HG12 | 14:YF:275[D]:ILE:HB | 1.68 | 0.75 |
| 13:YB:572[C]:ILE:HD12 | 15:ZA:29[C]:VAL:HG22 | 1.69 | 0.75 |
| 7:AI:13:SER:HB2 | 7:AJ:18:PHE:HA | 1.67 | 0.74 |
| 2:BJ:27:ASP:O | 2:BJ:34:TYR:OH | 2.05 | 0.74 |
| 2:C:933:ILE:HG12 | 2:C:935:LYS:H | 1.52 | 0.74 |
| 7:FE:228:ILE:HB | 7:FF:228:ILE:HD11 | 1.69 | 0.74 |
| 5:HD:84:GLY:O | 5:HD:86:VAL:N | 2.20 | 0.74 |
| 5:K:362:GLU:HG3 | 5:K:367:GLU:HB2 | 1.69 | 0.74 |
| 13:YA:61[B]:ILE:HG22 | 13:YB:76[B]:PRO:HA | 1.68 | 0.74 |
| 14:YD:250[A]:ASN:HD21 | 14:YD:272[A]:GLU:HB2 | 1.52 | 0.74 |
| 14:YD:250[F]:ASN:HD21 | 14:YD:272[F]:GLU:HB2 | 1.52 | 0.74 |
| 14:YD:41[A]:ARG:NH2 | 14:YD:341[A]:GLU:OE2 | 2.19 | 0.74 |
| 14:YF:30[D]:GLU:OE2 | 14:YF:32[D]:ALA:N | 2.19 | 0.74 |
| 14:YF:41[D]:ARG:NH2 | 14:YF:341[D]:GLU:OE2 | 2.19 | 0.74 |
| 5:AD:326:MET:HG3 | 5:AD:327:PRO:HD3 | 1.68 | 0.74 |
| 6:AG:87:TYR:HB2 | 6:AG:181:GLU:HB2 | 1.67 | 0.74 |
| 7:AJ:27:PRO:HA | 7:AJ:29:ILE:HD11 | 1.68 | 0.74 |
| 3:CB:195:PRO:HD3 | 3:CB:223:TRP:CD1 | 2.22 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:196:ARG:CZ | 7:DC:5:THR:HG23 | 2.16 | 0.74 |
| 6:FC:87:TYR:HB2 | 6:FC:181:GLU:HB2 | 1.67 | 0.74 |
| 7:FF:78:PRO:HB3 | 7:FG:66:VAL:HA | 1.68 | 0.74 |
| 7:O:445:HIS:NE2 | 7:Q:445:HIS:CE1 | 2.55 | 0.74 |
| 13:YB:232[A]:ASN:HB3 | 13:YC:407[A]:PRO:HB3 | 1.69 | 0.74 |
| 14:YE:250[D]:ASN:HD21 | 14:YE:272[D]:GLU:HB2 | 1.52 | 0.74 |
| 14:YF:253[C]:ILE:HG12 | 14:YF:275[C]:ILE:HB | 1.68 | 0.74 |
| 2:Z:27:ASP:O | 2:Z:34:TYR:OH | 2.05 | 0.74 |
| 2:Z:933:ILE:HG12 | 2:Z:935:LYS:H | 1.52 | 0.74 |
| 15:ZA:26[C]:GLN:HE22 | 15:ZA:29[C]:VAL:N | 1.85 | 0.74 |
| 2:BJ:39:ALA:HB3 | 2:BJ:79:ILE:HB | 1.69 | 0.74 |
| 2:BJ:928:GLU:HG3 | 2:BJ:929:TYR:H | 1.50 | 0.74 |
| 2:C:761:GLU:O | 2:C:765:GLY:N | 2.21 | 0.74 |
| 5:CF:299:ILE:O | 5:CF:301:GLY:N | 2.20 | 0.74 |
| 6:CI:70:ILE:HG12 | 6:CJ:73:ASN:HA | 1.69 | 0.74 |
| 1:GD:290:ASP:OD1 | 1:GD:291:THR:N | 2.19 | 0.74 |
| 3:GH:195:PRO:HD3 | 3:GH:223:TRP:CD1 | 2.22 | 0.74 |
| 13:YA:184[E]:GLU:HG2 | 13:YA:203[E]:GLY:HA3 | 1.69 | 0.74 |
| 14:YD:143[D]:ARG:HB3 | 14:YD:146[D]:LEU:HD12 | 1.69 | 0.74 |
| 14:YD:41[B]:ARG:NH2 | 14:YD:341[B]:GLU:OE2 | 2.19 | 0.74 |
| 14:YE:143[B]:ARG:HB3 | 14:YE:146[B]:LEU:HD12 | 1.69 | 0.74 |
| 14:YF:250[B]:ASN:HD21 | 14:YF:272[B]:GLU:HB2 | 1.52 | 0.74 |
| 4:AA:113:ASN:HD22 | 4:AB:103:LEU:HD21 | 1.51 | 0.74 |
| 2:GF:438:GLY:O | 2:GF:439:LYS:HG2 | 1.86 | 0.74 |
| 5:HC:326:MET:HG3 | 5:HC:327:PRO:HD3 | 1.68 | 0.74 |
| 5:HD:362:GLU:HG3 | 5:HD:367:GLU:HB2 | 1.69 | 0.74 |
| 8:IB:74:MET:HA | 8:IB:152:THR:HG22 | 1.68 | 0.74 |
| 7:O:212:PRO:HB2 | 7:P:203:THR:HG22 | 1.69 | 0.74 |
| 13:YA:337[D]:GLU:HG2 | 13:YA:342[D]:GLU:HA | 1.70 | 0.74 |
| 13:YB:397[F]:SER:OG | 13:YC:405[F]:ASP:OD1 | 2.04 | 0.74 |
| 13:YB:90[C]:TRP:NE1 | 14:YE:175[C]:GLU:OE1 | 2.19 | 0.74 |
| 14:YE:41[C]:ARG:NH2 | 14:YE:341[C]:GLU:OE2 | 2.19 | 0.74 |
| 14:YE:41[F]:ARG:NH2 | 14:YE:341[F]:GLU:OE2 | 2.19 | 0.74 |
| 14:YF:250[C]:ASN:HD21 | 14:YF:272[C]:GLU:HB2 | 1.52 | 0.74 |
| 7:AJ:191:VAL:O | 7:BA:189:GLY:N | 2.20 | 0.74 |
| 8:BB:74:MET:HA | 8:BB:152:THR:HG22 | 1.68 | 0.74 |
| 5:CF:180:VAL:HG11 | 5:CF:186:TYR:HB2 | 1.70 | 0.74 |
| 2:EC:69:PHE:CZ | 2:EC:71:ASP:HB2 | 2.21 | 0.74 |
| 5:EI:299:ILE:O | 5:EI:301:GLY:N | 2.20 | 0.74 |
| 8:FI:74:MET:HA | 8:FI:152:THR:HG22 | 1.68 | 0.74 |
| 5:K:261:ARG:HB2 | 5:K:383:ILE:HB | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:57:ILE:HG22 | 7:Q:55:LYS:HB3 | 1.70 | 0.74 |
| 11:V:186:ARG:HG3 | 11:V:187:ILE:HG12 | 1.68 | 0.74 |
| 13:YA:61[E]:ILE:HG23 | 13:YB:60[E]:PRO:HD3 | 1.70 | 0.74 |
| 13:YB:184[A]:GLU:HG2 | 13:YB:203[A]:GLY:HA3 | 1.69 | 0.74 |
| 13:YB:90[B]:TRP:NE1 | 14:YE:175[B]:GLU:OE1 | 2.19 | 0.74 |
| 13:YC:184[E]:GLU:HG2 | 13:YC:203[E]:GLY:HA3 | 1.69 | 0.74 |
| 14:YD:41[E]:ARG:NH2 | 14:YD:341[E]:GLU:OE2 | 2.19 | 0.74 |
| 14:YE:253[E]:ILE:HG12 | 14:YE:275[E]:ILE:HB | 1.68 | 0.74 |
| 14:YF:190[C]:GLN:HG2 | 14:YF:195[C]:VAL:HG22 | 1.70 | 0.74 |
| 13:YB:572[A]:ILE:HD12 | 15:ZA:29[A]:VAL:HG22 | 1.68 | 0.74 |
| 8:DF:74:MET:HA | 8:DF:152:THR:HG22 | 1.68 | 0.74 |
| 1:EB:111:MET:HG2 | 1:EB:304:PRO:HB3 | 1.70 | 0.74 |
| 2:EC:200:TYR:OH | 2:EC:292:GLU:OE1 | 2.04 | 0.74 |
| 3:ED:149:ASP:OD2 | 3:ED:152:GLU:N | 2.17 | 0.74 |
| 5:I:321:ALA:HA | 5:I:358:VAL:HB | 1.68 | 0.74 |
| 1:Y:111:MET:HG2 | 1:Y:304:PRO:HB3 | 1.70 | 0.74 |
| 13:YB:232[B]:ASN:HB3 | 13:YC:407[B]:PRO:HB3 | 1.68 | 0.74 |
| 13:YB:337[B]:GLU:HG2 | 13:YB:342[B]:GLU:HA | 1.70 | 0.74 |
| 14:YE:143[E]:ARG:HB3 | 14:YE:146[E]:LEU:HD12 | 1.69 | 0.74 |
| 14:YF:143[F]:ARG:HB3 | 14:YF:146[F]:LEU:HD12 | 1.69 | 0.74 |
| 14:YF:190[D]:GLN:HG2 | 14:YF:195[D]:VAL:HG22 | 1.70 | 0.74 |
| 3:CB:282:LYS:NZ | 3:CB:287:ASP:O | 2.21 | 0.74 |
| 6:CI:13:ARG:HG2 | 6:CI:14:LEU:H | 1.50 | 0.74 |
| 2:EC:27:ASP:O | 2:EC:34:TYR:OH | 2.05 | 0.74 |
| 7:FE:24:ASN:ND2 | 7:FG:45:ASN:OD1 | 2.19 | 0.74 |
| 2:GF:69:PHE:CZ | 2:GF:71:ASP:HB2 | 2.21 | 0.74 |
| 6:HE:28:ASP:OD2 | 6:HF:60:HIS:NE2 | 2.20 | 0.74 |
| 1:X:256:TYR:HB3 | 1:Y:324:ARG:HH22 | 1.52 | 0.74 |
| 14:YD:190[C]:GLN:HG2 | 14:YD:195[C]:VAL:HG22 | 1.70 | 0.74 |
| 14:YE:143[A]:ARG:HB3 | 14:YE:146[A]:LEU:HD12 | 1.69 | 0.74 |
| 14:YE:250[B]:ASN:HD21 | 14:YE:272[B]:GLU:HB2 | 1.52 | 0.74 |
| 2:Z:761:GLU:O | 2:Z:765:GLY:N | 2.21 | 0.74 |
| 11:BF:46:ARG:HD2 | 11:BF:173:ALA:HB2 | 1.69 | 0.74 |
| 1:BI:111:MET:HG2 | 1:BI:304:PRO:HB3 | 1.70 | 0.74 |
| 1:BH:403:PRO:HA | 1:BI:364:THR:HG21 | 1.70 | 0.74 |
| 1:EB:180:ASP:HA | 1:EB:264:GLN:HE22 | 1.53 | 0.74 |
| 11:GB:46:ARG:HD2 | 11:GB:173:ALA:HB2 | 1.69 | 0.74 |
| 1:GE:180:ASP:HA | 1:GE:264:GLN:HE22 | 1.53 | 0.74 |
| 1:GE:576:ASP:OD1 | 1:GE:577:PHE:N | 2.21 | 0.74 |
| 5:I:285:LEU:HD11 | 5:I:375:PHE:HB2 | 1.68 | 0.74 |
| 7:P:191:VAL:O | 7:Q:189:GLY:N | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:180:ASP:HA | 1:Y:264:GLN:HE22 | 1.53 | 0.74 |
| 13:YA:184[F]:GLU:HG2 | 13:YA:203[F]:GLY:HA3 | 1.68 | 0.74 |
| 14:YD:143[C]:ARG:HB3 | 14:YD:146[C]:LEU:HD12 | 1.69 | 0.74 |
| 14:YD:143[A]:ARG:HB3 | 14:YD:146[A]:LEU:HD12 | 1.69 | 0.74 |
| 14:YD:190[A]:GLN:HG2 | 14:YD:195[A]:VAL:HG22 | 1.70 | 0.74 |
| 14:YD:250[E]:ASN:HD21 | 14:YD:272[E]:GLU:HB2 | 1.52 | 0.74 |
| 14:YF:143[E]:ARG:HB3 | 14:YF:146[E]:LEU:HD12 | 1.69 | 0.74 |
| 1:B:180:ASP:HA | 1:B:264:GLN:HE22 | 1.53 | 0.74 |
| 2:BJ:333:ASN:HB2 | 4:CC:18:ALA:HA | 1.68 | 0.74 |
| 2:BJ:69:PHE:CZ | 2:BJ:71:ASP:HB2 | 2.21 | 0.74 |
| 2:BJ:803:SER:O | 2:BJ:806:LYS:N | 2.20 | 0.74 |
| 12:DJ:185:VAL:HG23 | 12:DJ:186:THR:HG23 | 1.70 | 0.74 |
| 7:FF:27:PRO:HA | 7:FF:29:ILE:HD11 | 1.68 | 0.74 |
| 2:GF:200:TYR:OH | 2:GF:292:GLU:OE1 | 2.04 | 0.74 |
| 7:HH:228:ILE:HB | 7:HI:228:ILE:HD11 | 1.70 | 0.74 |
| 5:K:84:GLY:O | 5:K:86:VAL:N | 2.20 | 0.74 |
| 7:O:132:ARG:NH1 | 7:Q:126:ASN:OD1 | 2.19 | 0.74 |
| 13:YB:184[D]:GLU:HG2 | 13:YB:203[D]:GLY:HA3 | 1.69 | 0.74 |
| 13:YB:397[A]:SER:OG | 13:YC:405[A]:ASP:OD1 | 2.04 | 0.74 |
| 13:YB:399[A]:HIS:CD2 | 13:YC:403[A]:PHE:HB3 | 2.23 | 0.74 |
| 13:YB:399[F]:HIS:CD2 | 13:YC:403[F]:PHE:HB3 | 2.23 | 0.74 |
| 13:YB:232[F]:ASN:HB3 | 13:YC:407[F]:PRO:HB3 | 1.69 | 0.74 |
| 14:YD:100[B]:LYS:NZ | 14:YF:215[B]:GLU:OE1 | 2.21 | 0.74 |
| 14:YD:250[D]:ASN:HD21 | 14:YD:272[D]:GLU:HB2 | 1.52 | 0.74 |
| 14:YE:190[E]:GLN:HG2 | 14:YE:195[E]:VAL:HG22 | 1.70 | 0.74 |
| 14:YE:190[F]:GLN:HG2 | 14:YE:195[F]:VAL:HG22 | 1.70 | 0.74 |
| 14:YF:143[C]:ARG:HB3 | 14:YF:146[C]:LEU:HD12 | 1.69 | 0.74 |
| 14:YF:250[A]:ASN:HD21 | 14:YF:272[A]:GLU:HB2 | 1.52 | 0.74 |
| 13:YB:572[D]:ILE:HD12 | 15:ZA:29[D]:VAL:HG22 | 1.69 | 0.74 |
| 1:A:555:ILE:HG22 | 1:A:590:TYR:H | 1.53 | 0.74 |
| 2:BJ:41:THR:OG1 | 2:BJ:77:THR:OG1 | 2.06 | 0.74 |
| 5:FA:261:ARG:HB2 | 5:FA:383:ILE:HB | 1.68 | 0.74 |
| 7:FF:166:GLN:NE2 | 7:FG:151:LEU:O | 2.21 | 0.74 |
| 7:HI:57:ILE:HG22 | 7:HJ:55:LYS:HB3 | 1.70 | 0.74 |
| 5:J:188:VAL:HG11 | 5:K:129:ARG:HE | 1.53 | 0.74 |
| 5:I:200:LEU:HB2 | 7:Q:5:THR:HG21 | 1.70 | 0.74 |
| 8:R:74:MET:HA | 8:R:152:THR:HG22 | 1.68 | 0.74 |
| 13:YB:184[F]:GLU:HG2 | 13:YB:203[F]:GLY:HA3 | 1.68 | 0.74 |
| 13:YB:370[D]:ASN:HD21 | 13:YB:372[D]:SER:HB3 | 1.53 | 0.74 |
| 13:YC:337[E]:GLU:HG2 | 13:YC:342[E]:GLU:HA | 1.70 | 0.74 |
| 13:YB:232[E]:ASN:HB3 | 13:YC:407[E]:PRO:HB3 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:190[B]:GLN:HG2 | 14:YD:195[B]:VAL:HG22 | 1.70 | 0.74 |
| 14:YE:143[D]:ARG:HB3 | 14:YE:146[D]:LEU:HD12 | 1.69 | 0.74 |
| 14:YE:190[A]:GLN:HG2 | 14:YE:195[A]:VAL:HG22 | 1.70 | 0.74 |
| 14:YF:143[B]:ARG:HB3 | 14:YF:146[B]:LEU:HD12 | 1.69 | 0.74 |
| 14:YF:41[A]:ARG:NH2 | 14:YF:341[A]:GLU:OE2 | 2.19 | 0.74 |
| 15:ZA:26[F]:GLN:HE22 | 15:ZA:29[F]:VAL:N | 1.85 | 0.74 |
| 5:AC:285:LEU:HD11 | 5:AC:375:PHE:HB2 | 1.68 | 0.73 |
| 5:AD:326:MET:HE1 | 5:AE:264:ARG:N | 2.03 | 0.73 |
| 7:AI:212:PRO:HB2 | 7:AJ:203:THR:HG22 | 1.70 | 0.73 |
| 1:B:455:PHE:HD1 | 1:B:639:LEU:HD12 | 1.50 | 0.73 |
| 1:BI:180:ASP:HA | 1:BI:264:GLN:HE22 | 1.53 | 0.73 |
| 2:C:258:LYS:NZ | 2:C:292:GLU:OE2 | 2.21 | 0.73 |
| 5:CG:34:TYR:OH | 5:CG:40:GLY:O | 2.03 | 0.73 |
| 5:CG:188:VAL:HG11 | 5:CH:129:ARG:HE | 1.53 | 0.73 |
| 7:DC:191:VAL:O | 7:DD:189:GLY:N | 2.20 | 0.73 |
| 1:EA:156:ASP:H | 1:EA:161:TYR:HB3 | 1.53 | 0.73 |
| 1:EB:325:ILE:O | 1:EB:329:GLY:N | 2.15 | 0.73 |
| 5:EI:180:VAL:HG11 | 5:EI:186:TYR:HB2 | 1.70 | 0.73 |
| 5:FA:34:TYR:O | 5:FA:38:GLY:N | 2.20 | 0.73 |
| 5:FA:290:SER:HA | 5:FA:371:PHE:HB3 | 1.70 | 0.73 |
| 1:GD:555:ILE:HG22 | 1:GD:590:TYR:H | 1.53 | 0.73 |
| 5:HB:321:ALA:HA | 5:HB:358:VAL:HB | 1.68 | 0.73 |
| 5:J:196:ARG:NH2 | 7:Q:9:VAL:HG12 | 2.03 | 0.73 |
| 5:K:34:TYR:O | 5:K:38:GLY:N | 2.20 | 0.73 |
| 7:O:401:ARG:HB3 | 7:Q:399:PHE:HE1 | 1.53 | 0.73 |
| 13:YB:76[E]:PRO:HB3 | 13:YB:98[E]:GLY:HA2 | 1.70 | 0.73 |
| 14:YD:143[F]:ARG:HB3 | 14:YD:146[F]:LEU:HD12 | 1.69 | 0.73 |
| 14:YD:190[F]:GLN:HG2 | 14:YD:195[F]:VAL:HG22 | 1.70 | 0.73 |
| 13:YB:90[F]:TRP:NE1 | 14:YE:175[F]:GLU:OE1 | 2.20 | 0.73 |
| 5:AC:321:ALA:HA | 5:AC:358:VAL:HB | 1.68 | 0.73 |
| 5:AE:84:GLY:O | 5:AE:86:VAL:N | 2.20 | 0.73 |
| 7:AJ:166:GLN:NE2 | 7:BA:151:LEU:O | 2.22 | 0.73 |
| 12:BG:185:VAL:HG23 | 12:BG:186:THR:HG23 | 1.70 | 0.73 |
| 1:BI:70:PHE:CE2 | 2:BJ:686:LEU:HB3 | 2.22 | 0.73 |
| 2:C:27:ASP:O | 2:C:34:TYR:OH | 2.06 | 0.73 |
| 6:CJ:87:TYR:HB2 | 6:CJ:181:GLU:HB2 | 1.67 | 0.73 |
| 7:DC:448:ALA:N | 7:DD:485:ASN:OD1 | 2.22 | 0.73 |
| 1:EB:494:THR:HG21 | 1:EB:603:TYR:HA | 1.69 | 0.73 |
| 2:EC:761:GLU:O | 2:EC:765:GLY:N | 2.21 | 0.73 |
| 7:FE:20:PRO:HD3 | 7:FE:29:ILE:HG21 | 1.70 | 0.73 |
| 7:HH:170:ILE:O | 7:HH:174:ALA:N | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:212:PRO:HB2 | 7:HI:203:THR:HG22 | 1.70 | 0.73 |
| 7:HI:448:ALA:N | 7:HJ:485:ASN:OD1 | 2.21 | 0.73 |
| 5:I:299:ILE:O | 5:I:301:GLY:N | 2.20 | 0.73 |
| 5:J:84:GLY:O | 5:J:86:VAL:N | 2.19 | 0.73 |
| 11:V:2:LEU:O | 11:V:5:PHE:N | 2.21 | 0.73 |
| 11:V:46:ARG:HD2 | 11:V:173:ALA:HB2 | 1.69 | 0.73 |
| 13:YB:370[A]:ASN:HD21 | 13:YB:372[A]:SER:HB3 | 1.53 | 0.73 |
| 13:YC:337[F]:GLU:HG2 | 13:YC:342[F]:GLU:HA | 1.70 | 0.73 |
| 14:YE:190[D]:GLN:HG2 | 14:YE:195[D]:VAL:HG22 | 1.70 | 0.73 |
| 14:YF:190[E]:GLN:HG2 | 14:YF:195[E]:VAL:HG22 | 1.70 | 0.73 |
| 14:YF:250[F]:ASN:HD21 | 14:YF:272[F]:GLU:HB2 | 1.52 | 0.73 |
| 15:ZA:26[B]:GLN:HE22 | 15:ZA:29[B]:VAL:N | 1.86 | 0.73 |
| 13:YB:572[B]:ILE:HD12 | 15:ZA:29[B]:VAL:HG22 | 1.69 | 0.73 |
| 5:AE:196:ARG:CZ | 7:AJ:5:THR:HG23 | 2.18 | 0.73 |
| 7:AI:20:PRO:HD3 | 7:AI:29:ILE:HG21 | 1.70 | 0.73 |
| 1:BI:494:THR:HG21 | 1:BI:603:TYR:HA | 1.69 | 0.73 |
| 2:BJ:926:PRO:HG3 | 2:BJ:969:TYR:HE2 | 1.53 | 0.73 |
| 1:EA:256:TYR:HB3 | 1:EB:324:ARG:HH22 | 1.53 | 0.73 |
| 12:GC:185:VAL:HG23 | 12:GC:186:THR:HG23 | 1.70 | 0.73 |
| 1:GE:111:MET:HG2 | 1:GE:304:PRO:HB3 | 1.70 | 0.73 |
| 1:GE:455:PHE:HD1 | 1:GE:639:LEU:HD12 | 1.50 | 0.73 |
| 5:HD:290:SER:HA | 5:HD:371:PHE:HB3 | 1.70 | 0.73 |
| 7:HJ:101:SER:O | 7:HJ:120:LYS:NZ | 2.16 | 0.73 |
| 5:I:180:VAL:HG11 | 5:I:186:TYR:HB2 | 1.70 | 0.73 |
| 12:W:185:VAL:HG23 | 12:W:186:THR:HG23 | 1.70 | 0.73 |
| 13:YB:337[A]:GLU:HG2 | 13:YB:342[A]:GLU:HA | 1.70 | 0.73 |
| 13:YB:399[E]:HIS:CD2 | 13:YC:403[E]:PHE:HB3 | 2.23 | 0.73 |
| 14:YE:250[F]:ASN:HD21 | 14:YE:272[F]:GLU:HB2 | 1.52 | 0.73 |
| 14:YF:250[D]:ASN:HD21 | 14:YF:272[D]:GLU:HB2 | 1.52 | 0.73 |
| 7:AI:399:PHE:CE1 | 7:AJ:401:ARG:HB3 | 2.21 | 0.73 |
| 1:B:111:MET:HG2 | 1:B:304:PRO:HB3 | 1.70 | 0.73 |
| 1:BI:576:ASP:OD1 | 1:BI:577:PHE:N | 2.21 | 0.73 |
| 2:C:400:ASP:OD2 | 2:C:404:TYR:OH | 2.06 | 0.73 |
| 7:DC:27:PRO:HA | 7:DC:29:ILE:HD11 | 1.68 | 0.73 |
| 7:DD:101:SER:O | 7:DD:120:LYS:NZ | 2.16 | 0.73 |
| 2:EC:400:ASP:OD2 | 2:EC:404:TYR:OH | 2.06 | 0.73 |
| 3:EE:282:LYS:NZ | 3:EE:287:ASP:O | 2.21 | 0.73 |
| 2:EC:985:GLU:N | 5:EJ:12:ASP:OD2 | 2.20 | 0.73 |
| 7:FE:132:ARG:NH1 | 7:FG:126:ASN:OD1 | 2.20 | 0.73 |
| 2:GF:258:LYS:NZ | 2:GF:292:GLU:OE2 | 2.21 | 0.73 |
| 7:HH:20:PRO:HD3 | 7:HH:29:ILE:HG21 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:20:PRO:HD3 | 7:O:29:ILE:HG21 | 1.70 | 0.73 |
| 7:O:66:VAL:HA | 7:Q:78:PRO:HB3 | 1.71 | 0.73 |
| 13:YC:184[B]:GLU:HG2 | 13:YC:203[B]:GLY:HA3 | 1.69 | 0.73 |
| 13:YC:184[C]:GLU:HG2 | 13:YC:203[C]:GLY:HA3 | 1.69 | 0.73 |
| 14:YD:100[F]:LYS:NZ | 14:YF:215[F]:GLU:OE1 | 2.22 | 0.73 |
| 14:YD:250[B]:ASN:HD21 | 14:YD:272[B]:GLU:HB2 | 1.52 | 0.73 |
| 14:YF:190[B]:GLN:HG2 | 14:YF:195[B]:VAL:HG22 | 1.70 | 0.73 |
| 14:YF:250[E]:ASN:HD21 | 14:YF:272[E]:GLU:HB2 | 1.52 | 0.73 |
| 2:Z:400:ASP:OD2 | 2:Z:404:TYR:OH | 2.06 | 0.73 |
| 7:AI:445:HIS:NE2 | 7:BA:445:HIS:CE1 | 2.56 | 0.73 |
| 2:BJ:323:ARG:HB3 | 2:BJ:362:LYS:HD2 | 1.71 | 0.73 |
| 5:CF:359:GLU:N | 5:CF:370:HIS:O | 2.22 | 0.73 |
| 5:CG:326:MET:HE1 | 5:CH:264:ARG:N | 2.04 | 0.73 |
| 7:DB:126:ASN:OD1 | 7:DC:132:ARG:NH1 | 2.21 | 0.73 |
| 7:DB:132:ARG:NH1 | 7:DD:126:ASN:OD1 | 2.21 | 0.73 |
| 2:EC:258:LYS:NZ | 2:EC:292:GLU:OE2 | 2.21 | 0.73 |
| 5:EI:339:GLU:HG2 | 6:FC:173:THR:HB | 1.70 | 0.73 |
| 5:FA:186:TYR:OH | 5:FA:191:ILE:HA | 1.89 | 0.73 |
| 6:FB:28:ASP:OD2 | 6:FC:60:HIS:NE2 | 2.20 | 0.73 |
| 7:FE:18:PHE:HA | 7:FG:13:SER:HB2 | 1.70 | 0.73 |
| 2:GF:27:ASP:O | 2:GF:34:TYR:OH | 2.05 | 0.73 |
| 1:GE:70:PHE:CE2 | 2:GF:686:LEU:HB3 | 2.23 | 0.73 |
| 4:GJ:50:VAL:HG12 | 4:GJ:51:ALA:H | 1.53 | 0.73 |
| 5:HD:34:TYR:O | 5:HD:38:GLY:N | 2.20 | 0.73 |
| 7:HH:401:ARG:HB3 | 7:HJ:399:PHE:HE1 | 1.54 | 0.73 |
| 7:HH:24:ASN:ND2 | 7:HJ:41:PRO:HA | 2.00 | 0.73 |
| 5:I:265:LEU:HB3 | 5:I:281:TYR:HB3 | 1.71 | 0.73 |
| 5:J:214:SER:OG | 5:J:222:LEU:O | 2.06 | 0.73 |
| 13:YB:522[E]:VAL:HA | 13:YC:514[E]:VAL:O | 1.89 | 0.73 |
| 13:YB:522[D]:VAL:HA | 13:YC:514[D]:VAL:O | 1.89 | 0.73 |
| 2:Z:41:THR:OG1 | 2:Z:77:THR:OG1 | 2.06 | 0.73 |
| 5:AC:299:ILE:O | 5:AC:301:GLY:N | 2.20 | 0.73 |
| 5:AD:188:VAL:HG11 | 5:AE:129:ARG:HE | 1.53 | 0.73 |
| 1:BH:156:ASP:H | 1:BH:161:TYR:HB3 | 1.54 | 0.73 |
| 5:CH:261:ARG:HB2 | 5:CH:383:ILE:HB | 1.68 | 0.73 |
| 7:DB:20:PRO:HD3 | 7:DB:29:ILE:HG21 | 1.70 | 0.73 |
| 2:EC:323:ARG:HB3 | 2:EC:362:LYS:HD2 | 1.71 | 0.73 |
| 7:FE:401:ARG:HB3 | 7:FG:399:PHE:HE1 | 1.52 | 0.73 |
| 5:HC:214:SER:OG | 5:HC:222:LEU:O | 2.06 | 0.73 |
| 5:HD:318:GLN:NE2 | 6:HF:4:LEU:O | 2.21 | 0.73 |
| 5:HD:339:GLU:HB3 | 6:HE:172:SER:O | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HF:70:ILE:HG12 | 6:HG:73:ASN:HA | 1.71 | 0.73 |
| 7:HH:66:VAL:HA | 7:HJ:78:PRO:HB3 | 1.71 | 0.73 |
| 13:YA:184[A]:GLU:HG2 | 13:YA:203[A]:GLY:HA3 | 1.69 | 0.73 |
| 13:YA:337[C]:GLU:HG2 | 13:YA:342[C]:GLU:HA | 1.70 | 0.73 |
| 13:YB:221[A]:LEU:HD12 | 13:YB:229[A]:ILE:HG13 | 1.71 | 0.73 |
| 13:YB:370[F]:ASN:HD21 | 13:YB:372[F]:SER:HB3 | 1.53 | 0.73 |
| 13:YB:90[A]:TRP:NE1 | 14:YE:175[A]:GLU:OE1 | 2.20 | 0.73 |
| 13:YB:58[A]:ILE:HG12 | 13:YB:97[A]:LEU:HD22 | 1.71 | 0.73 |
| 13:YC:184[D]:GLU:HG2 | 13:YC:203[D]:GLY:HA3 | 1.69 | 0.73 |
| 14:YE:215[D]:GLU:OE1 | 14:YF:100[D]:LYS:NZ | 2.22 | 0.73 |
| 14:YE:250[A]:ASN:HD21 | 14:YE:272[A]:GLU:HB2 | 1.52 | 0.73 |
| 14:YE:250[C]:ASN:HD21 | 14:YE:272[C]:GLU:HB2 | 1.53 | 0.73 |
| 5:AD:215:PRO:HG3 | 5:AD:226:ASP:HB2 | 1.70 | 0.73 |
| 7:AI:228:ILE:HB | 7:AJ:228:ILE:HD11 | 1.71 | 0.73 |
| 7:AI:220:SER:OG | 7:BA:228:ILE:O | 2.06 | 0.73 |
| 2:BJ:200:TYR:OH | 2:BJ:292:GLU:OE1 | 2.04 | 0.73 |
| 2:C:803:SER:O | 2:C:806:LYS:N | 2.20 | 0.73 |
| 5:EI:359:GLU:N | 5:EI:370:HIS:O | 2.22 | 0.73 |
| 7:P:457:LEU:HD21 | 5:EJ:412:PRO:HG3 | 1.69 | 0.73 |
| 5:EJ:84:GLY:O | 5:EJ:86:VAL:N | 2.19 | 0.73 |
| 7:HI:82:ALA:O | 7:HI:86:SER:N | 2.22 | 0.73 |
| 12:IF:185:VAL:HG23 | 12:IF:186:THR:HG23 | 1.70 | 0.73 |
| 7:O:228:ILE:HB | 7:P:228:ILE:HD11 | 1.71 | 0.73 |
| 1:A:435:TRP:HA | 1:X:152:ILE:HD11 | 1.69 | 0.73 |
| 1:X:156:ASP:H | 1:X:161:TYR:HB3 | 1.53 | 0.73 |
| 13:YA:337[A]:GLU:HG2 | 13:YA:342[A]:GLU:HA | 1.70 | 0.73 |
| 13:YB:337[D]:GLU:HG2 | 13:YB:342[D]:GLU:HA | 1.70 | 0.73 |
| 13:YB:370[E]:ASN:HD21 | 13:YB:372[E]:SER:HB3 | 1.54 | 0.73 |
| 13:YC:337[B]:GLU:HG2 | 13:YC:342[B]:GLU:HA | 1.70 | 0.73 |
| 2:Z:926:PRO:HG3 | 2:Z:969:TYR:HE2 | 1.53 | 0.73 |
| 5:AC:73:SER:HB3 | 5:AC:101:THR:HG21 | 1.71 | 0.73 |
| 1:BH:555:ILE:HB | 1:BH:592:ILE:HD11 | 1.71 | 0.73 |
| 2:C:926:PRO:HG3 | 2:C:969:TYR:HE2 | 1.53 | 0.73 |
| 2:C:985:GLU:N | 5:J:12:ASP:OD2 | 2.20 | 0.73 |
| 2:BJ:985:GLU:N | 5:CG:12:ASP:OD2 | 2.22 | 0.73 |
| 5:CG:214:SER:OG | 5:CG:222:LEU:O | 2.06 | 0.73 |
| 1:EB:576:ASP:OD1 | 1:EB:577:PHE:N | 2.21 | 0.73 |
| 1:EB:70:PHE:CE2 | 2:EC:686:LEU:HB3 | 2.23 | 0.73 |
| 5:EJ:214:SER:OG | 5:EJ:222:LEU:O | 2.06 | 0.73 |
| 1:GD:156:ASP:H | 1:GD:161:TYR:HB3 | 1.54 | 0.73 |
| 1:GD:555:ILE:HB | 1:GD:592:ILE:HD11 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:41:THR:OG1 | 2:GF:77:THR:OG1 | 2.06 | 0.73 |
| 5:HB:265:LEU:HB3 | 5:HB:281:TYR:HB3 | 1.70 | 0.73 |
| 7:HH:18:PHE:HA | 7:HJ:13:SER:HB2 | 1.71 | 0.73 |
| 5:K:186:TYR:OH | 5:K:191:ILE:HA | 1.89 | 0.73 |
| 5:K:196:ARG:CZ | 7:P:5:THR:HG23 | 2.18 | 0.73 |
| 1:Y:72:ASN:OD1 | 1:Y:73:ALA:N | 2.22 | 0.73 |
| 13:YA:184[B]:GLU:HG2 | 13:YA:203[B]:GLY:HA3 | 1.69 | 0.73 |
| 13:YB:522[C]:VAL:HA | 13:YC:514[C]:VAL:O | 1.89 | 0.73 |
| 14:YD:190[D]:GLN:HG2 | 14:YD:195[D]:VAL:HG22 | 1.70 | 0.73 |
| 14:YD:250[C]:ASN:HD21 | 14:YD:272[C]:GLU:HB2 | 1.52 | 0.73 |
| 14:YE:283[D]:TYR:O | 14:YE:286[D]:MET:HB2 | 1.89 | 0.73 |
| 14:YF:190[F]:GLN:HG2 | 14:YF:195[F]:VAL:HG22 | 1.70 | 0.73 |
| 2:Z:258:LYS:NZ | 2:Z:292:GLU:OE2 | 2.21 | 0.73 |
| 1:A:256:TYR:HB3 | 1:B:324:ARG:HH22 | 1.53 | 0.73 |
| 1:B:70:PHE:CE2 | 2:C:686:LEU:HB3 | 2.23 | 0.73 |
| 1:BH:555:ILE:HG22 | 1:BH:590:TYR:H | 1.53 | 0.73 |
| 2:C:323:ARG:HB3 | 2:C:362:LYS:HD2 | 1.71 | 0.73 |
| 2:C:41:THR:OG1 | 2:C:77:THR:OG1 | 2.06 | 0.73 |
| 1:EA:555:ILE:HB | 1:EA:592:ILE:HD11 | 1.71 | 0.73 |
| 5:FA:362:GLU:HG3 | 5:FA:367:GLU:HB2 | 1.69 | 0.73 |
| 1:GE:72:ASN:OD1 | 1:GE:73:ALA:N | 2.22 | 0.73 |
| 2:GF:323:ARG:HB3 | 2:GF:362:LYS:HD2 | 1.71 | 0.73 |
| 2:EC:174:HIS:NE2 | 3:GH:227:ASP:OD2 | 2.21 | 0.73 |
| 13:YA:76[E]:PRO:HB3 | 13:YA:98[E]:GLY:HA2 | 1.70 | 0.73 |
| 13:YB:232[D]:ASN:HB3 | 13:YC:407[D]:PRO:HB3 | 1.69 | 0.73 |
| 13:YB:337[E]:GLU:HG2 | 13:YB:342[E]:GLU:HA | 1.70 | 0.73 |
| 13:YB:370[C]:ASN:HD21 | 13:YB:372[C]:SER:HB3 | 1.53 | 0.73 |
| 13:YB:572[F]:ILE:HD12 | 15:ZA:29[F]:VAL:HG22 | 1.69 | 0.73 |
| 13:YB:399[D]:HIS:CD2 | 13:YC:403[D]:PHE:HB3 | 2.23 | 0.73 |
| 14:YD:143[B]:ARG:HB3 | 14:YD:146[B]:LEU:HD12 | 1.69 | 0.73 |
| 14:YE:190[C]:GLN:HG2 | 14:YE:195[C]:VAL:HG22 | 1.70 | 0.73 |
| 14:YF:190[A]:GLN:HG2 | 14:YF:195[A]:VAL:HG22 | 1.70 | 0.73 |
| 1:A:156:ASP:H | 1:A:161:TYR:HB3 | 1.54 | 0.73 |
| 5:AE:362:GLU:HG3 | 5:AE:367:GLU:HB2 | 1.69 | 0.73 |
| 8:BC:74:MET:HA | 8:BC:152:THR:HG22 | 1.68 | 0.73 |
| 2:BJ:761:GLU:O | 2:BJ:765:GLY:N | 2.21 | 0.73 |
| 2:C:771:ILE:HD13 | 2:C:840:ARG:HD3 | 1.71 | 0.73 |
| 7:FE:212:PRO:HB2 | 7:FF:203:THR:HG22 | 1.71 | 0.73 |
| 7:FG:101:SER:O | 7:FG:120:LYS:NZ | 2.16 | 0.73 |
| 1:GE:338:ARG:NH1 | 2:GF:738:LYS:O | 2.21 | 0.73 |
| 2:GF:926:PRO:HG3 | 2:GF:969:TYR:HE2 | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:29:ILE:HG22 | 7:HI:30:THR:H | 1.53 | 0.73 |
| 7:O:13:SER:HB2 | 7:P:18:PHE:HA | 1.69 | 0.73 |
| 1:Y:70:PHE:CE2 | 2:Z:686:LEU:HB3 | 2.24 | 0.73 |
| 13:YA:337[F]:GLU:HG2 | 13:YA:342[F]:GLU:HA | 1.70 | 0.73 |
| 13:YC:337[D]:GLU:HG2 | 13:YC:342[D]:GLU:HA | 1.70 | 0.73 |
| 13:YB:522[F]:VAL:HA | 13:YC:514[F]:VAL:O | 1.89 | 0.73 |
| 14:YD:283[D]:TYR:O | 14:YD:286[D]:MET:HB2 | 1.89 | 0.73 |
| 14:YF:283[B]:TYR:O | 14:YF:286[B]:MET:HB2 | 1.89 | 0.73 |
| 5:AC:359:GLU:N | 5:AC:370:HIS:O | 2.22 | 0.72 |
| 1:B:72:ASN:OD1 | 1:B:73:ALA:N | 2.22 | 0.72 |
| 2:BJ:258:LYS:NZ | 2:BJ:292:GLU:OE2 | 2.21 | 0.72 |
| 7:DC:29:ILE:HG22 | 7:DC:30:THR:H | 1.54 | 0.72 |
| 1:EA:555:ILE:HG22 | 1:EA:590:TYR:H | 1.53 | 0.72 |
| 5:EI:200:LEU:HB2 | 7:FG:5:THR:HG21 | 1.70 | 0.72 |
| 5:FA:285:LEU:HD11 | 5:FA:375:PHE:HB2 | 1.71 | 0.72 |
| 7:FF:82:ALA:O | 7:FF:86:SER:N | 2.22 | 0.72 |
| 2:GF:400:ASP:OD2 | 2:GF:404:TYR:OH | 2.06 | 0.72 |
| 2:GF:761:GLU:O | 2:GF:765:GLY:N | 2.21 | 0.72 |
| 2:GF:771:ILE:HD13 | 2:GF:840:ARG:HD3 | 1.71 | 0.72 |
| 2:GF:803:SER:O | 2:GF:806:LYS:N | 2.20 | 0.72 |
| 5:I:326:MET:HE1 | 5:J:264:ARG:HB3 | 1.71 | 0.72 |
| 7:P:166:GLN:NE2 | 7:Q:151:LEU:O | 2.21 | 0.72 |
| 7:Q:9:VAL:HG23 | 7:Q:10:SER:H | 1.54 | 0.72 |
| 1:X:334:GLU:HG2 | 2:Z:735:TYR:CE1 | 2.24 | 0.72 |
| 1:X:555:ILE:HG22 | 1:X:590:TYR:H | 1.53 | 0.72 |
| 13:YA:221[D]:LEU:HD12 | 13:YA:229[D]:ILE:HG13 | 1.71 | 0.72 |
| 13:YA:221[D]:LEU:HD11 | 13:YA:236[D]:ILE:HD11 | 1.71 | 0.72 |
| 13:YB:572[E]:ILE:HD12 | 15:ZA:29[E]:VAL:HG22 | 1.69 | 0.72 |
| 13:YC:221[F]:LEU:HD11 | 13:YC:236[F]:ILE:HD11 | 1.71 | 0.72 |
| 14:YD:283[F]:TYR:O | 14:YD:286[F]:MET:HB2 | 1.89 | 0.72 |
| 14:YE:143[F]:ARG:HB3 | 14:YE:146[F]:LEU:HD12 | 1.69 | 0.72 |
| 14:YE:190[B]:GLN:HG2 | 14:YE:195[B]:VAL:HG22 | 1.70 | 0.72 |
| 14:YF:143[D]:ARG:HB3 | 14:YF:146[D]:LEU:HD12 | 1.69 | 0.72 |
| 14:YF:283[D]:TYR:O | 14:YF:286[D]:MET:HB2 | 1.89 | 0.72 |
| 1:A:555:ILE:HB | 1:A:592:ILE:HD11 | 1.71 | 0.72 |
| 5:AC:180:VAL:HG11 | 5:AC:186:TYR:HB2 | 1.70 | 0.72 |
| 5:AD:214:SER:OG | 5:AD:222:LEU:O | 2.06 | 0.72 |
| 1:A:403:PRO:HA | 1:B:364:THR:HG21 | 1.71 | 0.72 |
| 7:AI:18:PHE:HA | 7:BA:13:SER:HB2 | 1.71 | 0.72 |
| 1:BI:240:GLU:N | 1:BI:240:GLU:OE1 | 2.22 | 0.72 |
| 7:DC:166:GLN:NE2 | 7:DD:151:LEU:O | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:265:LEU:HB3 | 5:EI:281:TYR:HB3 | 1.70 | 0.72 |
| 2:EC:228:ARG:HH22 | 5:FA:559:PRO:HB3 | 1.52 | 0.72 |
| 3:GH:282:LYS:NZ | 3:GH:287:ASP:O | 2.21 | 0.72 |
| 1:Y:576:ASP:OD1 | 1:Y:577:PHE:N | 2.21 | 0.72 |
| 13:YB:232[C]:ASN:HB3 | 13:YC:407[C]:PRO:HB3 | 1.69 | 0.72 |
| 13:YC:221[E]:LEU:HD12 | 13:YC:229[E]:ILE:HG13 | 1.71 | 0.72 |
| 13:YC:58[A]:ILE:HG12 | 13:YC:97[A]:LEU:HD22 | 1.71 | 0.72 |
| 13:YC:58[D]:ILE:HG12 | 13:YC:97[D]:LEU:HD22 | 1.71 | 0.72 |
| 14:YD:283[B]:TYR:O | 14:YD:286[B]:MET:HB2 | 1.89 | 0.72 |
| 2:Z:323:ARG:HB3 | 2:Z:362:LYS:HD2 | 1.71 | 0.72 |
| 15:ZA:26[A]:GLN:HE22 | 15:ZA:29[A]:VAL:N | 1.85 | 0.72 |
| 4:AA:10:ILE:HD11 | 4:AA:31:ILE:HD11 | 1.72 | 0.72 |
| 5:AC:397:ASP:OD1 | 5:AC:398:GLU:N | 2.23 | 0.72 |
| 5:AE:186:TYR:OH | 5:AE:191:ILE:HA | 1.89 | 0.72 |
| 6:AF:12:SER:HB3 | 6:AH:6:ASN:HB3 | 1.71 | 0.72 |
| 7:BA:9:VAL:HG23 | 7:BA:10:SER:H | 1.54 | 0.72 |
| 1:BI:72:ASN:OD1 | 1:BI:73:ALA:N | 2.22 | 0.72 |
| 5:CF:397:ASP:OD1 | 5:CF:398:GLU:N | 2.23 | 0.72 |
| 5:CG:180:VAL:HG11 | 5:CG:186:TYR:HB2 | 1.72 | 0.72 |
| 5:CH:186:TYR:OH | 5:CH:191:ILE:HA | 1.89 | 0.72 |
| 5:CH:290:SER:HA | 5:CH:371:PHE:HB3 | 1.70 | 0.72 |
| 7:DC:82:ALA:O | 7:DC:86:SER:N | 2.22 | 0.72 |
| 8:DE:74:MET:HA | 8:DE:152:THR:HG22 | 1.68 | 0.72 |
| 1:BI:76:TYR:OH | 11:DI:29:PHE:O | 2.07 | 0.72 |
| 11:DI:46:ARG:HD2 | 11:DI:173:ALA:HB2 | 1.69 | 0.72 |
| 3:E:282:LYS:NZ | 3:E:287:ASP:O | 2.21 | 0.72 |
| 5:HB:180:VAL:HG11 | 5:HB:186:TYR:HB2 | 1.70 | 0.72 |
| 11:IE:2:LEU:O | 11:IE:5:PHE:N | 2.21 | 0.72 |
| 13:YB:184[E]:GLU:HG2 | 13:YB:203[E]:GLY:HA3 | 1.69 | 0.72 |
| 13:YC:337[C]:GLU:HG2 | 13:YC:342[C]:GLU:HA | 1.70 | 0.72 |
| 13:YC:50[D]:GLU:CD | 13:YC:50[D]:GLU:H | 1.91 | 0.72 |
| 13:YB:522[B]:VAL:HA | 13:YC:514[B]:VAL:O | 1.89 | 0.72 |
| 14:YD:100[D]:LYS:NZ | 14:YF:215[D]:GLU:OE1 | 2.23 | 0.72 |
| 14:YD:190[E]:GLN:HG2 | 14:YD:195[E]:VAL:HG22 | 1.70 | 0.72 |
| 14:YE:283[A]:TYR:O | 14:YE:286[A]:MET:HB2 | 1.89 | 0.72 |
| 14:YE:283[B]:TYR:O | 14:YE:286[B]:MET:HB2 | 1.89 | 0.72 |
| 14:YE:283[F]:TYR:O | 14:YE:286[F]:MET:HB2 | 1.90 | 0.72 |
| 14:YF:283[E]:TYR:O | 14:YF:286[E]:MET:HB2 | 1.89 | 0.72 |
| 14:YF:283[F]:TYR:O | 14:YF:286[F]:MET:HB2 | 1.89 | 0.72 |
| 5:AE:290:SER:HA | 5:AE:371:PHE:HB3 | 1.70 | 0.72 |
| 3:CB:260:GLU:OE1 | 3:CB:260:GLU:N | 2.21 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DC:49:ASP:O | 7:DC:57:ILE:N | 2.22 | 0.72 |
| 3:E:260:GLU:N | 3:E:260:GLU:OE1 | 2.21 | 0.72 |
| 4:EG:10:ILE:HD11 | 4:EG:31:ILE:HD11 | 1.71 | 0.72 |
| 5:EI:84:GLY:O | 5:EI:86:VAL:N | 2.22 | 0.72 |
| 7:FF:29:ILE:HG22 | 7:FF:30:THR:H | 1.53 | 0.72 |
| 7:FF:71:ASN:HB2 | 7:HJ:365:GLY:HA2 | 1.72 | 0.72 |
| 3:GG:282:LYS:NZ | 3:GG:289:ASN:OD1 | 2.21 | 0.72 |
| 3:GH:202:ARG:HB3 | 3:GH:209:VAL:HG21 | 1.72 | 0.72 |
| 4:GJ:64:THR:HA | 4:HA:84:ARG:HE | 1.54 | 0.72 |
| 4:H:50:VAL:HG12 | 4:H:51:ALA:H | 1.53 | 0.72 |
| 7:HI:166:GLN:NE2 | 7:HJ:151:LEU:O | 2.22 | 0.72 |
| 7:HH:445:HIS:NE2 | 7:HJ:445:HIS:CE1 | 2.56 | 0.72 |
| 5:J:326:MET:HE1 | 5:K:264:ARG:N | 2.03 | 0.72 |
| 5:K:290:SER:HA | 5:K:371:PHE:HB3 | 1.70 | 0.72 |
| 13:YA:58[D]:ILE:HG12 | 13:YA:97[D]:LEU:HD22 | 1.71 | 0.72 |
| 13:YB:221[B]:LEU:HD11 | 13:YB:236[B]:ILE:HD11 | 1.72 | 0.72 |
| 5:AE:318:GLN:NE2 | 6:AG:4:LEU:O | 2.23 | 0.72 |
| 1:B:576:ASP:OD1 | 1:B:577:PHE:N | 2.21 | 0.72 |
| 11:BF:2:LEU:O | 11:BF:5:PHE:N | 2.21 | 0.72 |
| 11:BF:2:LEU:HD11 | 11:BF:71:TRP:CE2 | 2.25 | 0.72 |
| 2:BJ:400:ASP:OD2 | 2:BJ:404:TYR:OH | 2.06 | 0.72 |
| 2:BJ:935:LYS:NZ | 2:BJ:936:LEU:HD13 | 2.05 | 0.72 |
| 11:DI:2:LEU:HD11 | 11:DI:71:TRP:CE2 | 2.25 | 0.72 |
| 5:EJ:180:VAL:HG11 | 5:EJ:186:TYR:HB2 | 1.72 | 0.72 |
| 7:FE:57:ILE:HG22 | 7:FF:55:LYS:HB3 | 1.72 | 0.72 |
| 2:GF:195:SER:OG | 2:GF:196:GLU:OE1 | 2.07 | 0.72 |
| 5:HB:89:TYR:CE1 | 5:HB:139:ALA:HA | 2.25 | 0.72 |
| 5:HB:397:ASP:OD1 | 5:HB:398:GLU:N | 2.23 | 0.72 |
| 5:HC:215:PRO:HG3 | 5:HC:226:ASP:HB2 | 1.71 | 0.72 |
| 5:HD:186:TYR:OH | 5:HD:191:ILE:HA | 1.89 | 0.72 |
| 11:IE:2:LEU:HD11 | 11:IE:71:TRP:CE2 | 2.25 | 0.72 |
| 1:Y:240:GLU:N | 1:Y:240:GLU:OE1 | 2.22 | 0.72 |
| 13:YB:337[F]:GLU:HG2 | 13:YB:342[F]:GLU:HA | 1.70 | 0.72 |
| 13:YB:399[B]:HIS:CD2 | 13:YC:403[B]:PHE:HB3 | 2.23 | 0.72 |
| 13:YB:57[A]:VAL:HG11 | 13:YB:76[A]:PRO:HD3 | 1.72 | 0.72 |
| 7:AJ:29:ILE:HG22 | 7:AJ:30:THR:H | 1.53 | 0.72 |
| 2:C:195:SER:OG | 2:C:196:GLU:OE1 | 2.07 | 0.72 |
| 5:CF:73:SER:HB3 | 5:CF:101:THR:HG21 | 1.71 | 0.72 |
| 5:CF:290:SER:HB2 | 5:CF:370:HIS:HA | 1.72 | 0.72 |
| 5:CG:84:GLY:O | 5:CG:86:VAL:N | 2.19 | 0.72 |
| 5:CH:362:GLU:HG3 | 5:CH:367:GLU:HB2 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:202:ARG:HB3 | 3:E:209:VAL:HG21 | 1.72 | 0.72 |
| 4:EG:69:LYS:NZ | 4:EH:103:LEU:O | 2.20 | 0.72 |
| 1:GE:139:SER:OG | 1:GE:141:ASN:OD1 | 2.04 | 0.72 |
| 5:HB:290:SER:HB2 | 5:HB:370:HIS:HA | 1.72 | 0.72 |
| 5:HC:251:VAL:O | 5:HD:161:ASN:ND2 | 2.21 | 0.72 |
| 7:HJ:9:VAL:HG23 | 7:HJ:10:SER:H | 1.54 | 0.72 |
| 2:C:228:ARG:HH22 | 5:K:559:PRO:HB3 | 1.55 | 0.72 |
| 13:YA:337[B]:GLU:HG2 | 13:YA:342[B]:GLU:HA | 1.70 | 0.72 |
| 13:YA:337[E]:GLU:HG2 | 13:YA:342[E]:GLU:HA | 1.70 | 0.72 |
| 13:YA:57[D]:VAL:HG11 | 13:YA:76[D]:PRO:HD3 | 1.72 | 0.72 |
| 13:YB:370[B]:ASN:HD21 | 13:YB:372[B]:SER:HB3 | 1.54 | 0.72 |
| 13:YC:221[D]:LEU:HD12 | 13:YC:229[D]:ILE:HG13 | 1.71 | 0.72 |
| 13:YC:337[A]:GLU:HG2 | 13:YC:342[A]:GLU:HA | 1.70 | 0.72 |
| 14:YD:283[C]:TYR:O | 14:YD:286[C]:MET:HB2 | 1.90 | 0.72 |
| 5:AD:180:VAL:HG11 | 5:AD:186:TYR:HB2 | 1.72 | 0.72 |
| 5:CG:215:PRO:HG3 | 5:CG:226:ASP:HB2 | 1.70 | 0.72 |
| 5:CH:285:LEU:HD11 | 5:CH:375:PHE:HB2 | 1.71 | 0.72 |
| 8:DE:56:ARG:HD3 | 8:FH:64:ARG:HD3 | 1.71 | 0.72 |
| 1:EA:334:GLU:HG2 | 2:EC:735:TYR:CE1 | 2.25 | 0.72 |
| 5:EI:397:ASP:OD1 | 5:EI:398:GLU:N | 2.23 | 0.72 |
| 5:EI:89:TYR:CE1 | 5:EI:139:ALA:HA | 2.25 | 0.72 |
| 5:FA:84:GLY:O | 5:FA:86:VAL:N | 2.20 | 0.72 |
| 8:BC:56:ARG:NH2 | 8:FI:96:GLY:O | 2.23 | 0.72 |
| 4:G:64:THR:HA | 4:H:84:ARG:HE | 1.55 | 0.72 |
| 4:GI:163:SER:HB3 | 4:HA:168:PHE:HA | 1.72 | 0.72 |
| 5:HB:84:GLY:O | 5:HB:86:VAL:N | 2.22 | 0.72 |
| 1:X:555:ILE:HB | 1:X:592:ILE:HD11 | 1.71 | 0.72 |
| 13:YB:399[C]:HIS:CD2 | 13:YC:403[C]:PHE:HB3 | 2.23 | 0.72 |
| 4:AA:50:VAL:HG12 | 4:AA:51:ALA:H | 1.53 | 0.72 |
| 4:AB:50:VAL:HG12 | 4:AB:51:ALA:H | 1.53 | 0.72 |
| 5:AD:34:TYR:OH | 5:AD:40:GLY:O | 2.03 | 0.72 |
| 7:AJ:57:ILE:HG22 | 7:BA:55:LYS:HB3 | 1.70 | 0.72 |
| 7:AI:199:VAL:HA | 7:BA:212:PRO:HB3 | 1.72 | 0.72 |
| 2:BJ:664:PHE:HB2 | 9:DG:15:MET:HB2 | 1.70 | 0.72 |
| 2:C:333:ASN:HB2 | 4:F:18:ALA:HA | 1.70 | 0.72 |
| 2:BJ:228:ARG:HH22 | 5:CH:559:PRO:HB3 | 1.54 | 0.72 |
| 3:D:282:LYS:NZ | 3:D:289:ASN:OD1 | 2.21 | 0.72 |
| 2:EC:195:SER:OG | 2:EC:196:GLU:OE1 | 2.07 | 0.72 |
| 5:EI:290:SER:HB2 | 5:EI:370:HIS:HA | 1.72 | 0.72 |
| 5:EI:264:ARG:HB3 | 5:FA:326:MET:HE1 | 1.70 | 0.72 |
| 7:FE:445:HIS:NE2 | 7:FG:445:HIS:CE1 | 2.56 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:334:GLU:HG2 | 2:GF:735:TYR:CE1 | 2.25 | 0.72 |
| 5:HB:359:GLU:N | 5:HB:370:HIS:O | 2.22 | 0.72 |
| 6:FB:77:VAL:HG23 | 7:HI:167:GLN:HE21 | 1.55 | 0.72 |
| 1:B:174:ARG:O | 11:V:145:GLN:NE2 | 2.22 | 0.72 |
| 13:YA:373[E]:ARG:HA | 13:YA:373[E]:ARG:HE | 1.55 | 0.72 |
| 13:YA:50[B]:GLU:CD | 13:YA:50[B]:GLU:H | 1.91 | 0.72 |
| 13:YB:221[B]:LEU:HD12 | 13:YB:229[B]:ILE:HG13 | 1.71 | 0.72 |
| 13:YB:57[E]:VAL:HG12 | 13:YB:96[E]:VAL:HB | 1.71 | 0.72 |
| 13:YB:522[A]:VAL:HA | 13:YC:514[A]:VAL:O | 1.89 | 0.72 |
| 13:YC:76[E]:PRO:HB3 | 13:YC:98[E]:GLY:HA2 | 1.70 | 0.72 |
| 2:Z:374:LYS:NZ | 2:Z:499:GLU:OE2 | 2.18 | 0.72 |
| 1:A:144:ASN:O | 1:A:169:GLN:NE2 | 2.23 | 0.72 |
| 5:AD:490:TRP:NE1 | 5:AD:500:ALA:O | 2.23 | 0.72 |
| 1:BH:563:VAL:HG22 | 1:BH:611:LEU:HD21 | 1.72 | 0.72 |
| 1:BI:102:SER:H | 1:BI:194:ARG:HH12 | 1.38 | 0.72 |
| 2:C:236:THR:HG22 | 2:C:515:ASN:HB3 | 1.72 | 0.72 |
| 1:EA:144:ASN:O | 1:EA:169:GLN:NE2 | 2.23 | 0.72 |
| 2:EC:41:THR:OG1 | 2:EC:77:THR:OG1 | 2.06 | 0.72 |
| 4:F:50:VAL:HG12 | 4:F:51:ALA:H | 1.53 | 0.72 |
| 7:FF:191:VAL:O | 7:FG:189:GLY:N | 2.22 | 0.72 |
| 11:GB:2:LEU:O | 11:GB:5:PHE:N | 2.21 | 0.72 |
| 5:I:397:ASP:OD1 | 5:I:398:GLU:N | 2.23 | 0.72 |
| 5:J:180:VAL:HG11 | 5:J:186:TYR:HB2 | 1.72 | 0.72 |
| 7:P:82:ALA:O | 7:P:86:SER:N | 2.22 | 0.72 |
| 7:P:448:ALA:N | 7:Q:485:ASN:OD1 | 2.21 | 0.72 |
| 7:Q:371:ASP:OD1 | 7:Q:526:LYS:NZ | 2.23 | 0.72 |
| 11:V:190:LYS:HE3 | 14:YE:24[F]:SER:O | 1.90 | 0.72 |
| 13:YB:221[A]:LEU:HD11 | 13:YB:236[A]:ILE:HD11 | 1.72 | 0.72 |
| 13:YB:373[C]:ARG:HE | 13:YB:373[C]:ARG:HA | 1.55 | 0.72 |
| 13:YC:221[A]:LEU:HD11 | 13:YC:236[A]:ILE:HD11 | 1.71 | 0.72 |
| 1:B:431:GLU:HG2 | 1:B:435:TRP:CE3 | 2.25 | 0.72 |
| 7:AI:66:VAL:HA | 7:BA:78:PRO:HB3 | 1.71 | 0.72 |
| 2:C:374:LYS:NZ | 2:C:499:GLU:OE2 | 2.18 | 0.72 |
| 7:DC:57:ILE:HG22 | 7:DD:55:LYS:HB3 | 1.70 | 0.72 |
| 7:DD:9:VAL:HG23 | 7:DD:10:SER:H | 1.54 | 0.72 |
| 1:EB:361:GLN:OE1 | 1:EB:362:THR:N | 2.23 | 0.72 |
| 2:EC:926:PRO:HG3 | 2:EC:969:TYR:HE2 | 1.53 | 0.72 |
| 5:EJ:326:MET:HE1 | 5:FA:264:ARG:N | 2.05 | 0.72 |
| 7:FF:40:SER:HB3 | 7:FG:24:ASN:HB2 | 1.71 | 0.72 |
| 7:FF:49:ASP:O | 7:FF:57:ILE:N | 2.22 | 0.72 |
| 5:HB:73:SER:HB3 | 5:HB:101:THR:HG21 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:490:TRP:NE1 | 5:HC:500:ALA:O | 2.23 | 0.72 |
| 5:HD:285:LEU:HD11 | 5:HD:375:PHE:HB2 | 1.71 | 0.72 |
| 5:I:316:ILE:HG23 | 5:J:315:GLY:HA3 | 1.72 | 0.72 |
| 7:P:366:THR:HG22 | 7:P:391:GLY:HA2 | 1.72 | 0.72 |
| 7:P:49:ASP:O | 7:P:57:ILE:N | 2.22 | 0.72 |
| 7:O:199:VAL:HA | 7:Q:212:PRO:HB3 | 1.71 | 0.72 |
| 13:YA:221[C]:LEU:HD11 | 13:YA:236[C]:ILE:HD11 | 1.72 | 0.72 |
| 13:YA:221[C]:LEU:HD12 | 13:YA:229[C]:ILE:HG13 | 1.72 | 0.72 |
| 13:YA:221[E]:LEU:HD11 | 13:YA:236[E]:ILE:HD11 | 1.72 | 0.72 |
| 13:YA:373[B]:ARG:HE | 13:YA:373[B]:ARG:HA | 1.55 | 0.72 |
| 13:YB:221[C]:LEU:HD11 | 13:YB:236[C]:ILE:HD11 | 1.72 | 0.72 |
| 13:YB:337[C]:GLU:HG2 | 13:YB:342[C]:GLU:HA | 1.70 | 0.72 |
| 13:YB:434[C]:THR:OG1 | 13:YC:430[C]:ARG:NH1 | 2.23 | 0.72 |
| 13:YC:373[E]:ARG:HA | 13:YC:373[E]:ARG:HE | 1.55 | 0.72 |
| 13:YC:373[F]:ARG:HA | 13:YC:373[F]:ARG:HE | 1.55 | 0.72 |
| 13:YC:373[C]:ARG:HE | 13:YC:373[C]:ARG:HA | 1.55 | 0.72 |
| 14:YD:143[E]:ARG:HB3 | 14:YD:146[E]:LEU:HD12 | 1.69 | 0.72 |
| 14:YD:283[E]:TYR:O | 14:YD:286[E]:MET:HB2 | 1.89 | 0.72 |
| 2:Z:935:LYS:NZ | 2:Z:936:LEU:HD13 | 2.05 | 0.72 |
| 1:A:563:VAL:HG22 | 1:A:611:LEU:HD21 | 1.72 | 0.71 |
| 5:AC:84:GLY:O | 5:AC:86:VAL:N | 2.22 | 0.71 |
| 6:AF:77:VAL:HG23 | 7:DC:167:GLN:HE21 | 1.55 | 0.71 |
| 5:CG:397:ASP:OD1 | 5:CG:398:GLU:N | 2.23 | 0.71 |
| 1:EB:240:GLU:OE1 | 1:EB:240:GLU:N | 2.22 | 0.71 |
| 1:EB:431:GLU:HG2 | 1:EB:435:TRP:CE3 | 2.25 | 0.71 |
| 1:EB:72:ASN:OD1 | 1:EB:73:ALA:N | 2.22 | 0.71 |
| 4:EG:50:VAL:HG12 | 4:EG:51:ALA:H | 1.53 | 0.71 |
| 4:EF:163:SER:HB3 | 4:EH:168:PHE:HA | 1.72 | 0.71 |
| 2:EC:1000:THR:HA | 5:EI:18:TYR:HA | 1.71 | 0.71 |
| 5:EI:234:GLN:HE22 | 7:FG:9:VAL:HG21 | 1.55 | 0.71 |
| 5:EJ:215:PRO:HG3 | 5:EJ:226:ASP:HB2 | 1.71 | 0.71 |
| 1:GE:431:GLU:HG2 | 1:GE:435:TRP:CE3 | 2.25 | 0.71 |
| 2:GF:985:GLU:N | 5:HC:12:ASP:OD2 | 2.21 | 0.71 |
| 7:HJ:371:ASP:OD1 | 7:HJ:526:LYS:NZ | 2.23 | 0.71 |
| 7:P:12:GLU:HB3 | 7:P:15:TYR:HB3 | 1.72 | 0.71 |
| 1:Y:361:GLN:OE1 | 1:Y:362:THR:N | 2.23 | 0.71 |
| 13:YB:373[B]:ARG:HE | 13:YB:373[B]:ARG:HA | 1.55 | 0.71 |
| 13:YB:373[F]:ARG:HE | 13:YB:373[F]:ARG:HA | 1.55 | 0.71 |
| 14:YE:283[C]:TYR:O | 14:YE:286[C]:MET:HB2 | 1.90 | 0.71 |
| 14:YF:283[A]:TYR:O | 14:YF:286[A]:MET:HB2 | 1.89 | 0.71 |
| 7:AJ:448:ALA:N | 7:BA:485:ASN:OD1 | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:236:THR:HG22 | 2:BJ:515:ASN:HB3 | 1.72 | 0.71 |
| 5:CF:265:LEU:HB3 | 5:CF:281:TYR:HB3 | 1.71 | 0.71 |
| 5:CF:339:GLU:HG2 | 6:CJ:173:THR:HB | 1.72 | 0.71 |
| 2:EC:935:LYS:NZ | 2:EC:936:LEU:HD13 | 2.05 | 0.71 |
| 4:EF:50:VAL:HG12 | 4:EF:51:ALA:H | 1.53 | 0.71 |
| 4:EH:50:VAL:HG12 | 4:EH:51:ALA:H | 1.53 | 0.71 |
| 4:EG:64:THR:HA | 4:EH:84:ARG:HE | 1.54 | 0.71 |
| 4:F:10:ILE:HD11 | 4:F:31:ILE:HD11 | 1.71 | 0.71 |
| 7:FE:448:ALA:N | 7:FF:485:ASN:OD1 | 2.23 | 0.71 |
| 7:FF:366:THR:HG22 | 7:FF:391:GLY:HA2 | 1.71 | 0.71 |
| 7:FG:9:VAL:HG23 | 7:FG:10:SER:H | 1.54 | 0.71 |
| 11:GB:2:LEU:HD11 | 11:GB:71:TRP:CE2 | 2.25 | 0.71 |
| 3:GH:260:GLU:N | 3:GH:260:GLU:OE1 | 2.21 | 0.71 |
| 4:GI:10:ILE:HD11 | 4:GI:31:ILE:HD11 | 1.71 | 0.71 |
| 4:GI:50:VAL:HG12 | 4:GI:51:ALA:H | 1.53 | 0.71 |
| 5:I:359:GLU:N | 5:I:370:HIS:O | 2.22 | 0.71 |
| 5:J:290:SER:HB2 | 5:J:370:HIS:HA | 1.73 | 0.71 |
| 1:Y:102:SER:H | 1:Y:194:ARG:HH12 | 1.38 | 0.71 |
| 13:YA:50[F]:GLU:H | 13:YA:50[F]:GLU:CD | 1.91 | 0.71 |
| 13:YA:76[B]:PRO:HA | 13:YC:61[B]:ILE:HG22 | 1.72 | 0.71 |
| 13:YC:221[E]:LEU:HD11 | 13:YC:236[E]:ILE:HD11 | 1.72 | 0.71 |
| 14:YF:143[A]:ARG:HB3 | 14:YF:146[A]:LEU:HD12 | 1.69 | 0.71 |
| 2:Z:803:SER:O | 2:Z:806:LYS:N | 2.20 | 0.71 |
| 7:AJ:82:ALA:O | 7:AJ:86:SER:N | 2.22 | 0.71 |
| 1:BI:431:GLU:HG2 | 1:BI:435:TRP:CE3 | 2.25 | 0.71 |
| 2:BJ:195:SER:OG | 2:BJ:196:GLU:OE1 | 2.07 | 0.71 |
| 1:BH:435:TRP:HA | 1:EA:152:ILE:HD11 | 1.71 | 0.71 |
| 1:EA:403:PRO:HA | 1:EB:364:THR:HG21 | 1.72 | 0.71 |
| 5:EJ:340:VAL:HG23 | 5:EJ:341:GLU:HG3 | 1.72 | 0.71 |
| 5:EJ:397:ASP:OD1 | 5:EJ:398:GLU:N | 2.23 | 0.71 |
| 7:FE:178:PRO:HB2 | 7:FE:180:GLU:HG2 | 1.73 | 0.71 |
| 7:FF:448:ALA:N | 7:FG:485:ASN:OD1 | 2.22 | 0.71 |
| 5:HC:180:VAL:HG11 | 5:HC:186:TYR:HB2 | 1.72 | 0.71 |
| 7:HI:12:GLU:HB3 | 7:HI:15:TYR:HB3 | 1.72 | 0.71 |
| 5:I:89:TYR:CE1 | 5:I:139:ALA:HA | 2.25 | 0.71 |
| 5:J:490:TRP:NE1 | 5:J:500:ALA:O | 2.23 | 0.71 |
| 13:YA:50[C]:GLU:CD | 13:YA:50[C]:GLU:H | 1.91 | 0.71 |
| 13:YB:221[D]:LEU:HD11 | 13:YB:236[D]:ILE:HD11 | 1.72 | 0.71 |
| 13:YB:373[E]:ARG:HA | 13:YB:373[E]:ARG:HE | 1.55 | 0.71 |
| 13:YC:221[A]:LEU:HD12 | 13:YC:229[A]:ILE:HG13 | 1.71 | 0.71 |
| 13:YB:434[E]:THR:OG1 | 13:YC:430[E]:ARG:NH1 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:57[A]:VAL:HG11 | 13:YC:76[A]:PRO:HD3 | 1.72 | 0.71 |
| 14:YD:215[F]:GLU:OE1 | 14:YE:100[F]:LYS:NZ | 2.23 | 0.71 |
| 14:YE:143[C]:ARG:HB3 | 14:YE:146[C]:LEU:HD12 | 1.69 | 0.71 |
| 14:YE:283[E]:TYR:O | 14:YE:286[E]:MET:HB2 | 1.89 | 0.71 |
| 4:AB:10:ILE:HD11 | 4:AB:31:ILE:HD11 | 1.71 | 0.71 |
| 5:AC:339:GLU:HG2 | 6:AG:173:THR:HB | 1.70 | 0.71 |
| 7:AI:366:THR:HG22 | 7:AI:391:GLY:HA2 | 1.73 | 0.71 |
| 7:AI:401:ARG:HB3 | 7:BA:399:PHE:HE1 | 1.54 | 0.71 |
| 1:B:139:SER:OG | 1:B:141:ASN:OD1 | 2.04 | 0.71 |
| 2:BJ:771:ILE:HD13 | 2:BJ:840:ARG:HD3 | 1.71 | 0.71 |
| 2:C:664:PHE:HB2 | 9:T:15:MET:HB2 | 1.71 | 0.71 |
| 5:CH:318:GLN:NE2 | 6:CJ:4:LEU:O | 2.24 | 0.71 |
| 2:BJ:474:GLU:HB3 | 3:EE:155:LYS:HE2 | 1.71 | 0.71 |
| 4:EF:10:ILE:HD11 | 4:EF:31:ILE:HD11 | 1.72 | 0.71 |
| 5:EJ:251:VAL:O | 5:FA:161:ASN:ND2 | 2.23 | 0.71 |
| 5:FA:305:ASN:HD21 | 5:FA:386:PHE:HB2 | 1.55 | 0.71 |
| 7:FG:371:ASP:OD1 | 7:FG:526:LYS:NZ | 2.23 | 0.71 |
| 8:DE:162:TRP:O | 8:FH:95:GLN:NE2 | 2.22 | 0.71 |
| 4:G:50:VAL:HG12 | 4:G:51:ALA:H | 1.53 | 0.71 |
| 1:GE:240:GLU:OE1 | 1:GE:240:GLU:N | 2.22 | 0.71 |
| 4:GJ:10:ILE:HD11 | 4:GJ:31:ILE:HD11 | 1.72 | 0.71 |
| 5:HC:594:THR:OG1 | 5:HD:517:GLY:N | 2.23 | 0.71 |
| 5:HB:407:TYR:CE1 | 5:HD:407:TYR:HB2 | 2.26 | 0.71 |
| 7:HI:40:SER:HB3 | 7:HJ:24:ASN:HB2 | 1.73 | 0.71 |
| 12:GC:142:ASN:ND2 | 10:ID:210:ASP:O | 2.24 | 0.71 |
| 7:O:18:PHE:HA | 7:Q:13:SER:HB2 | 1.72 | 0.71 |
| 13:YA:221[B]:LEU:HD12 | 13:YA:229[B]:ILE:HG13 | 1.71 | 0.71 |
| 13:YA:373[C]:ARG:HA | 13:YA:373[C]:ARG:HE | 1.55 | 0.71 |
| 13:YA:373[D]:ARG:HE | 13:YA:373[D]:ARG:HA | 1.56 | 0.71 |
| 13:YA:373[F]:ARG:HA | 13:YA:373[F]:ARG:HE | 1.55 | 0.71 |
| 13:YB:434[D]:THR:OG1 | 13:YC:430[D]:ARG:NH1 | 2.24 | 0.71 |
| 13:YB:434[F]:THR:OG1 | 13:YC:430[F]:ARG:NH1 | 2.23 | 0.71 |
| 13:YC:221[F]:LEU:HD12 | 13:YC:229[F]:ILE:HG13 | 1.72 | 0.71 |
| 13:YC:373[A]:ARG:HE | 13:YC:373[A]:ARG:HA | 1.56 | 0.71 |
| 13:YC:373[D]:ARG:HA | 13:YC:373[D]:ARG:HE | 1.56 | 0.71 |
| 13:YC:50[B]:GLU:H | 13:YC:50[B]:GLU:CD | 1.91 | 0.71 |
| 5:AC:265:LEU:HB3 | 5:AC:281:TYR:HB3 | 1.71 | 0.71 |
| 5:AD:290:SER:HB2 | 5:AD:370:HIS:HA | 1.73 | 0.71 |
| 6:AG:70:ILE:HG12 | 6:AH:73:ASN:HA | 1.73 | 0.71 |
| 7:BA:371:ASP:OD1 | 7:BA:526:LYS:NZ | 2.23 | 0.71 |
| 1:BH:256:TYR:HB3 | 1:BI:324:ARG:HH22 | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:CA:149:ASP:OD2 | 3:CA:152:GLU:N | 2.17 | 0.71 |
| 4:CE:50:VAL:HG12 | 4:CE:51:ALA:H | 1.53 | 0.71 |
| 11:DI:2:LEU:O | 11:DI:5:PHE:N | 2.21 | 0.71 |
| 2:BJ:529:SER:OG | 3:EE:233:GLN:OE1 | 2.09 | 0.71 |
| 2:GF:199:LEU:HB3 | 2:GF:212:SER:HB2 | 1.72 | 0.71 |
| 2:EC:188:ASN:OD1 | 3:GG:286:ASN:ND2 | 2.24 | 0.71 |
| 4:GJ:168:PHE:HA | 4:HA:163:SER:HB3 | 1.72 | 0.71 |
| 11:V:2:LEU:HD11 | 11:V:71:TRP:CE2 | 2.25 | 0.71 |
| 13:YA:221[A]:LEU:HD12 | 13:YA:229[A]:ILE:HG13 | 1.71 | 0.71 |
| 13:YA:221[F]:LEU:HD11 | 13:YA:236[F]:ILE:HD11 | 1.72 | 0.71 |
| 13:YC:57[D]:VAL:HG11 | 13:YC:76[D]:PRO:HD3 | 1.72 | 0.71 |
| 4:CD:50:VAL:HG12 | 4:CD:51:ALA:H | 1.53 | 0.71 |
| 3:D:149:ASP:OD2 | 3:D:152:GLU:N | 2.17 | 0.71 |
| 7:DC:366:THR:HG22 | 7:DC:391:GLY:HA2 | 1.71 | 0.71 |
| 2:EC:509:TYR:HB3 | 3:GH:229:LEU:HD23 | 1.73 | 0.71 |
| 3:EE:202:ARG:HB3 | 3:EE:209:VAL:HG21 | 1.72 | 0.71 |
| 1:A:152:ILE:HD11 | 1:GD:435:TRP:HA | 1.72 | 0.71 |
| 7:HH:178:PRO:HB2 | 7:HH:180:GLU:HG2 | 1.72 | 0.71 |
| 5:J:491:ASN:HD22 | 5:J:496:ASP:HB2 | 1.56 | 0.71 |
| 7:O:178:PRO:HB2 | 7:O:180:GLU:HG2 | 1.73 | 0.71 |
| 7:P:29:ILE:HG22 | 7:P:30:THR:H | 1.54 | 0.71 |
| 8:R:56:ARG:NH2 | 8:BB:96:GLY:O | 2.23 | 0.71 |
| 1:X:240:GLU:N | 1:X:240:GLU:OE1 | 2.24 | 0.71 |
| 13:YA:373[A]:ARG:HE | 13:YA:373[A]:ARG:HA | 1.56 | 0.71 |
| 13:YB:434[B]:THR:OG1 | 13:YC:430[B]:ARG:NH1 | 2.24 | 0.71 |
| 13:YB:554[F]:MET:HE2 | 13:YC:550[F]:TRP:CD1 | 2.25 | 0.71 |
| 13:YC:373[B]:ARG:HA | 13:YC:373[B]:ARG:HE | 1.55 | 0.71 |
| 13:YC:50[E]:GLU:CD | 13:YC:50[E]:GLU:H | 1.91 | 0.71 |
| 14:YD:283[A]:TYR:O | 14:YD:286[A]:MET:HB2 | 1.89 | 0.71 |
| 2:Z:968:ASP:HB3 | 2:Z:972:GLU:HG2 | 1.73 | 0.71 |
| 5:AC:290:SER:HB2 | 5:AC:370:HIS:HA | 1.72 | 0.71 |
| 7:AI:178:PRO:HB2 | 7:AI:180:GLU:HG2 | 1.72 | 0.71 |
| 1:BI:347:THR:O | 1:BI:350:SER:N | 2.24 | 0.71 |
| 5:CF:326:MET:HE1 | 5:CG:264:ARG:HB3 | 1.72 | 0.71 |
| 7:DB:178:PRO:HB2 | 7:DB:180:GLU:HG2 | 1.73 | 0.71 |
| 7:DB:228:ILE:HB | 7:DC:228:ILE:HD11 | 1.73 | 0.71 |
| 7:DC:513:ARG:N | 7:DD:441:GLN:O | 2.20 | 0.71 |
| 7:DB:445:HIS:NE2 | 7:DD:445:HIS:CE1 | 2.58 | 0.71 |
| 5:EI:73:SER:HB3 | 5:EI:101:THR:HG21 | 1.71 | 0.71 |
| 6:FD:90:PHE:HD2 | 6:FD:126:VAL:HG22 | 1.56 | 0.71 |
| 7:FF:333:THR:OG1 | 7:FF:335:ASN:OD1 | 2.08 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FF:100:TYR:OH | 7:FG:113:GLU:O | 2.05 | 0.71 |
| 2:GF:236:THR:HG22 | 2:GF:515:ASN:HB3 | 1.72 | 0.71 |
| 1:X:144:ASN:O | 1:X:169:GLN:NE2 | 2.23 | 0.71 |
| 13:YB:221[E]:LEU:HD12 | 13:YB:229[E]:ILE:HG13 | 1.71 | 0.71 |
| 13:YB:373[D]:ARG:HA | 13:YB:373[D]:ARG:HE | 1.56 | 0.71 |
| 13:YB:434[A]:THR:OG1 | 13:YC:430[A]:ARG:NH1 | 2.24 | 0.71 |
| 13:YC:221[B]:LEU:HD11 | 13:YC:236[B]:ILE:HD11 | 1.72 | 0.71 |
| 13:YC:221[D]:LEU:HD11 | 13:YC:236[D]:ILE:HD11 | 1.71 | 0.71 |
| 2:Z:195:SER:OG | 2:Z:196:GLU:OE1 | 2.07 | 0.71 |
| 5:AC:89:TYR:CE1 | 5:AC:139:ALA:HA | 2.25 | 0.71 |
| 1:B:102:SER:H | 1:B:194:ARG:HH12 | 1.37 | 0.71 |
| 7:BA:85:LEU:HG | 7:BA:86:SER:H | 1.56 | 0.71 |
| 1:BI:361:GLN:OE1 | 1:BI:362:THR:N | 2.23 | 0.71 |
| 2:C:935:LYS:NZ | 2:C:936:LEU:HD13 | 2.05 | 0.71 |
| 7:DD:85:LEU:HG | 7:DD:86:SER:H | 1.56 | 0.71 |
| 1:EA:231:ASP:OD2 | 1:EA:233:ASN:ND2 | 2.24 | 0.71 |
| 1:GD:231:ASP:OD2 | 1:GD:233:ASN:ND2 | 2.24 | 0.71 |
| 1:GE:347:THR:O | 1:GE:350:SER:N | 2.24 | 0.71 |
| 2:GF:935:LYS:NZ | 2:GF:936:LEU:HD13 | 2.05 | 0.71 |
| 5:HC:290:SER:HB2 | 5:HC:370:HIS:HA | 1.73 | 0.71 |
| 5:I:73:SER:HB3 | 5:I:101:THR:HG21 | 1.71 | 0.71 |
| 10:ID:214:ARG:HH12 | 12:IF:246:ARG:HH12 | 1.39 | 0.71 |
| 1:X:63:ASN:ND2 | 1:Y:60:LEU:HB3 | 2.06 | 0.71 |
| 13:YA:50[D]:GLU:H | 13:YA:50[D]:GLU:CD | 1.91 | 0.71 |
| 13:YB:221[F]:LEU:HD11 | 13:YB:236[F]:ILE:HD11 | 1.72 | 0.71 |
| 13:YB:58[D]:ILE:HG12 | 13:YB:97[D]:LEU:HD22 | 1.71 | 0.71 |
| 14:YF:283[C]:TYR:O | 14:YF:286[C]:MET:HB2 | 1.90 | 0.71 |
| 2:Z:771:ILE:HD13 | 2:Z:840:ARG:HD3 | 1.71 | 0.71 |
| 1:A:334:GLU:HG2 | 2:C:735:TYR:CE1 | 2.25 | 0.71 |
| 5:AD:84:GLY:O | 5:AD:86:VAL:N | 2.19 | 0.71 |
| 7:AJ:333:THR:OG1 | 7:AJ:335:ASN:OD1 | 2.08 | 0.71 |
| 5:AC:200:LEU:HB2 | 7:BA:5:THR:HG21 | 1.73 | 0.71 |
| 5:AD:196:ARG:NH2 | 7:BA:9:VAL:HG12 | 2.05 | 0.71 |
| 1:BI:23:GLY:H | 11:DI:26:THR:HG1 | 1.37 | 0.71 |
| 2:BJ:174:HIS:HD1 | 2:BJ:508:TYR:HH | 1.37 | 0.71 |
| 2:C:58:ASN:OD1 | 2:C:60:GLY:N | 2.23 | 0.71 |
| 5:CF:312:ARG:HG2 | 5:CF:317:LEU:HA | 1.73 | 0.71 |
| 5:CF:84:GLY:O | 5:CF:86:VAL:N | 2.22 | 0.71 |
| 5:CG:340:VAL:HG23 | 5:CG:341:GLU:HG3 | 1.72 | 0.71 |
| 6:FB:90:PHE:HD2 | 6:FB:126:VAL:HG22 | 1.56 | 0.71 |
| 7:FG:85:LEU:HG | 7:FG:86:SER:H | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:563:VAL:HG22 | 1:GD:611:LEU:HD21 | 1.72 | 0.71 |
| 7:HI:330:ARG:NH2 | 7:HI:336:GLU:OE2 | 2.22 | 0.71 |
| 7:HI:513:ARG:N | 7:HJ:441:GLN:O | 2.19 | 0.71 |
| 5:I:290:SER:HB2 | 5:I:370:HIS:HA | 1.72 | 0.71 |
| 7:O:96:GLY:O | 8:IA:56:ARG:NH2 | 320.64 | 0.71 |
| 5:J:215:PRO:HG3 | 5:J:226:ASP:HB2 | 1.71 | 0.71 |
| 6:N:90:PHE:HD2 | 6:N:126:VAL:HG22 | 1.56 | 0.71 |
| 1:X:403:PRO:HA | 1:Y:364:THR:HG21 | 1.73 | 0.71 |
| 1:Y:431:GLU:HG2 | 1:Y:435:TRP:CE3 | 2.25 | 0.71 |
| 13:YA:221[B]:LEU:HD11 | 13:YA:236[B]:ILE:HD11 | 1.72 | 0.71 |
| 13:YA:36[B]:PRO:HG3 | 13:YA:45[B]:MET:HB2 | 1.73 | 0.71 |
| 13:YC:36[E]:PRO:HG3 | 13:YC:45[E]:MET:HB2 | 1.73 | 0.71 |
| 1:A:231:ASP:OD2 | 1:A:233:ASN:ND2 | 2.24 | 0.71 |
| 5:AD:397:ASP:OD1 | 5:AD:398:GLU:N | 2.23 | 0.71 |
| 1:B:361:GLN:OE1 | 1:B:362:THR:N | 2.23 | 0.71 |
| 7:DB:66:VAL:HA | 7:DD:78:PRO:HB3 | 1.72 | 0.71 |
| 1:EA:563:VAL:HG22 | 1:EA:611:LEU:HD21 | 1.72 | 0.71 |
| 1:EB:102:SER:H | 1:EB:194:ARG:HH12 | 1.38 | 0.71 |
| 2:EC:303:ASN:OD1 | 2:EC:327:ARG:NH1 | 2.24 | 0.71 |
| 4:EH:10:ILE:HD11 | 4:EH:31:ILE:HD11 | 1.71 | 0.71 |
| 2:GF:174:HIS:HD1 | 2:GF:508:TYR:HH | 1.37 | 0.71 |
| 4:G:168:PHE:HA | 4:H:163:SER:HB3 | 1.73 | 0.71 |
| 4:HA:50:VAL:HG12 | 4:HA:51:ALA:H | 1.53 | 0.71 |
| 5:HB:241:THR:HG21 | 5:HD:200:LEU:HD13 | 1.72 | 0.71 |
| 13:YB:373[A]:ARG:HE | 13:YB:373[A]:ARG:HA | 1.56 | 0.71 |
| 14:YD:215[B]:GLU:OE1 | 14:YE:100[B]:LYS:NZ | 2.24 | 0.71 |
| 5:AC:326:MET:HE1 | 5:AD:264:ARG:HB3 | 1.73 | 0.70 |
| 1:BH:144:ASN:O | 1:BH:169:GLN:NE2 | 2.23 | 0.70 |
| 1:BH:66:TYR:CE1 | 1:BI:21:PHE:HB2 | 2.26 | 0.70 |
| 4:CC:50:VAL:HG12 | 4:CC:51:ALA:H | 1.53 | 0.70 |
| 5:CF:264:ARG:HB3 | 5:CH:326:MET:HE1 | 1.71 | 0.70 |
| 5:CG:490:TRP:NE1 | 5:CG:500:ALA:O | 2.23 | 0.70 |
| 7:DB:13:SER:HB2 | 7:DC:18:PHE:HA | 1.71 | 0.70 |
| 7:DC:333:THR:OG1 | 7:DC:335:ASN:OD1 | 2.08 | 0.70 |
| 1:EA:240:GLU:OE1 | 1:EA:240:GLU:N | 2.24 | 0.70 |
| 5:EI:312:ARG:HG2 | 5:EI:317:LEU:HA | 1.73 | 0.70 |
| 7:FE:66:VAL:HA | 7:FG:78:PRO:HB3 | 1.73 | 0.70 |
| 7:FF:330:ARG:NH2 | 7:FF:336:GLU:OE2 | 2.22 | 0.70 |
| 1:GD:144:ASN:O | 1:GD:169:GLN:NE2 | 2.23 | 0.70 |
| 3:GG:104:TYR:HB3 | 3:GG:166:SER:H | 1.56 | 0.70 |
| 5:HB:279:SER:HB2 | 5:HD:326:MET:HE3 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:366:THR:HG22 | 7:HI:391:GLY:HA2 | 1.72 | 0.70 |
| 11:V:190:LYS:HE3 | 14:YF:24[D]:SER:O | 1.90 | 0.70 |
| 13:YA:221[E]:LEU:HD12 | 13:YA:229[E]:ILE:HG13 | 1.71 | 0.70 |
| 13:YB:57[D]:VAL:HG11 | 13:YB:76[D]:PRO:HD3 | 1.72 | 0.70 |
| 2:Z:927:THR:N | 2:Z:985:GLU:OE2 | 2.24 | 0.70 |
| 7:AI:120:LYS:O | 7:AI:124:ALA:N | 2.24 | 0.70 |
| 7:AI:193:LEU:HD11 | 7:AJ:207:GLY:HA2 | 1.73 | 0.70 |
| 1:B:546:ASP:OD1 | 1:B:547:SER:N | 2.24 | 0.70 |
| 1:BH:231:ASP:OD2 | 1:BH:233:ASN:ND2 | 2.24 | 0.70 |
| 1:BH:334:GLU:HG2 | 2:BJ:735:TYR:CE1 | 2.26 | 0.70 |
| 2:BJ:374:LYS:NZ | 2:BJ:499:GLU:OE2 | 2.18 | 0.70 |
| 1:BI:403:PRO:HG3 | 2:BJ:885:PRO:HG3 | 1.72 | 0.70 |
| 2:C:199:LEU:HB3 | 2:C:212:SER:HB2 | 1.72 | 0.70 |
| 2:C:200:TYR:OH | 2:C:292:GLU:OE1 | 2.04 | 0.70 |
| 2:C:991:SER:O | 2:C:993:LEU:N | 2.24 | 0.70 |
| 4:CC:10:ILE:HD11 | 4:CC:31:ILE:HD11 | 1.71 | 0.70 |
| 4:CD:10:ILE:HD11 | 4:CD:31:ILE:HD11 | 1.71 | 0.70 |
| 7:DB:366:THR:HG22 | 7:DB:391:GLY:HA2 | 1.73 | 0.70 |
| 7:DD:229:LYS:HG3 | 7:DD:243:VAL:HG12 | 1.73 | 0.70 |
| 1:EB:338:ARG:NH1 | 2:EC:738:LYS:O | 2.22 | 0.70 |
| 2:EC:803:SER:O | 2:EC:806:LYS:N | 2.20 | 0.70 |
| 7:FG:229:LYS:HG3 | 7:FG:243:VAL:HG12 | 1.73 | 0.70 |
| 1:GD:240:GLU:N | 1:GD:240:GLU:OE1 | 2.24 | 0.70 |
| 5:HB:316:ILE:HG23 | 5:HC:315:GLY:HA3 | 1.73 | 0.70 |
| 7:HJ:85:LEU:HG | 7:HJ:86:SER:H | 1.56 | 0.70 |
| 5:K:318:GLN:NE2 | 6:M:4:LEU:O | 2.24 | 0.70 |
| 1:X:231:ASP:OD2 | 1:X:233:ASN:ND2 | 2.24 | 0.70 |
| 13:YB:221[D]:LEU:HD12 | 13:YB:229[D]:ILE:HG13 | 1.71 | 0.70 |
| 13:YC:169[E]:ASP:O | 13:YC:272[E]:SER:OG | 2.10 | 0.70 |
| 13:YC:221[C]:LEU:HD12 | 13:YC:229[C]:ILE:HG13 | 1.72 | 0.70 |
| 13:YC:221[B]:LEU:HD12 | 13:YC:229[B]:ILE:HG13 | 1.71 | 0.70 |
| 13:YC:221[C]:LEU:HD11 | 13:YC:236[C]:ILE:HD11 | 1.71 | 0.70 |
| 2:Z:174:HIS:HD1 | 2:Z:508:TYR:HH | 1.35 | 0.70 |
| 5:AD:340:VAL:HG23 | 5:AD:341:GLU:HG3 | 1.72 | 0.70 |
| 1:BI:139:SER:OG | 1:BI:141:ASN:OD1 | 2.04 | 0.70 |
| 2:C:303:ASN:OD1 | 2:C:327:ARG:NH1 | 2.24 | 0.70 |
| 4:CD:64:THR:HA | 4:CE:84:ARG:HE | 1.55 | 0.70 |
| 5:CF:89:TYR:CE1 | 5:CF:139:ALA:HA | 2.25 | 0.70 |
| 6:CI:90:PHE:HD2 | 6:CI:126:VAL:HG22 | 1.56 | 0.70 |
| 1:EA:435:TRP:HA | 1:GD:152:ILE:HD11 | 1.71 | 0.70 |
| 3:E:227:ASP:OD2 | 2:GF:174:HIS:NE2 | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:10:ILE:HD11 | 4:H:31:ILE:HD11 | 1.72 | 0.70 |
| 4:HA:10:ILE:HD11 | 4:HA:31:ILE:HD11 | 1.72 | 0.70 |
| 5:HD:305:ASN:HD21 | 5:HD:386:PHE:HB2 | 1.55 | 0.70 |
| 7:HH:220:SER:OG | 7:HJ:228:ILE:O | 2.06 | 0.70 |
| 7:HJ:229:LYS:HG3 | 7:HJ:243:VAL:HG12 | 1.73 | 0.70 |
| 5:HB:200:LEU:HB2 | 7:HJ:5:THR:HG21 | 1.73 | 0.70 |
| 7:P:167:GLN:HE21 | 6:HE:77:VAL:HG23 | 1.56 | 0.70 |
| 7:O:24:ASN:ND2 | 7:Q:41:PRO:HA | 2.01 | 0.70 |
| 1:Y:347:THR:O | 1:Y:350:SER:N | 2.24 | 0.70 |
| 13:YB:169[B]:ASP:O | 13:YB:272[B]:SER:OG | 2.10 | 0.70 |
| 13:YB:221[F]:LEU:HD12 | 13:YB:229[F]:ILE:HG13 | 1.72 | 0.70 |
| 14:YE:215[B]:GLU:OE1 | 14:YF:100[B]:LYS:NZ | 2.25 | 0.70 |
| 2:Z:411:LYS:HG3 | 2:Z:412:THR:HG22 | 1.73 | 0.70 |
| 1:A:195:ASN:OD1 | 1:A:352:ARG:NH1 | 2.24 | 0.70 |
| 5:AC:312:ARG:HG2 | 5:AC:317:LEU:HA | 1.73 | 0.70 |
| 1:BH:240:GLU:OE1 | 1:BH:240:GLU:N | 2.24 | 0.70 |
| 2:BJ:303:ASN:OD1 | 2:BJ:327:ARG:NH1 | 2.24 | 0.70 |
| 7:AJ:71:ASN:HB2 | 7:DD:365:GLY:HA2 | 1.73 | 0.70 |
| 3:ED:104:TYR:HB3 | 3:ED:166:SER:H | 1.56 | 0.70 |
| 5:EJ:290:SER:HB2 | 5:EJ:370:HIS:HA | 1.73 | 0.70 |
| 7:FE:120:LYS:O | 7:FE:124:ALA:N | 2.24 | 0.70 |
| 7:FF:12:GLU:HB3 | 7:FF:15:TYR:HB3 | 1.72 | 0.70 |
| 1:GD:256:TYR:HB3 | 1:GE:324:ARG:HH22 | 1.55 | 0.70 |
| 1:GD:403:PRO:HA | 1:GE:364:THR:HG21 | 1.72 | 0.70 |
| 2:GF:991:SER:O | 2:GF:993:LEU:N | 2.24 | 0.70 |
| 5:HC:397:ASP:OD1 | 5:HC:398:GLU:N | 2.23 | 0.70 |
| 7:HI:496:ARG:NH1 | 7:HI:501:THR:OG1 | 2.24 | 0.70 |
| 8:IA:88:TRP:CZ3 | 8:IA:134:PRO:HD3 | 2.26 | 0.70 |
| 6:M:52:ILE:HD11 | 6:N:15:ALA:HB2 | 1.74 | 0.70 |
| 7:O:120:LYS:O | 7:O:124:ALA:N | 2.24 | 0.70 |
| 7:Q:85:LEU:HG | 7:Q:86:SER:H | 1.56 | 0.70 |
| 13:YA:221[A]:LEU:HD11 | 13:YA:236[A]:ILE:HD11 | 1.72 | 0.70 |
| 13:YA:58[A]:ILE:HG12 | 13:YA:97[A]:LEU:HD22 | 1.71 | 0.70 |
| 13:YB:221[E]:LEU:HD11 | 13:YB:236[E]:ILE:HD11 | 1.72 | 0.70 |
| 13:YB:36[E]:PRO:HG3 | 13:YB:45[E]:MET:HB2 | 1.73 | 0.70 |
| 13:YB:61[E]:ILE:CG2 | 13:YC:59[E]:GLN:HA | 2.20 | 0.70 |
| 13:YC:50[F]:GLU:H | 13:YC:50[F]:GLU:CD | 1.91 | 0.70 |
| 14:YE:36[A]:THR:HG22 | 14:YE:37[A]:THR:HG23 | 1.73 | 0.70 |
| 2:Z:991:SER:O | 2:Z:993:LEU:N | 2.24 | 0.70 |
| 15:ZA:26[E]:GLN:HE22 | 15:ZA:29[E]:VAL:N | 1.86 | 0.70 |
| 1:A:240:GLU:OE1 | 1:A:240:GLU:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:285:LEU:HD11 | 5:AE:375:PHE:HB2 | 1.71 | 0.70 |
| 7:BA:229:LYS:HG3 | 7:BA:243:VAL:HG12 | 1.73 | 0.70 |
| 8:S:56:ARG:NH2 | 8:BC:96:GLY:O | 2.24 | 0.70 |
| 2:BJ:678:GLY:O | 2:BJ:684:ASN:ND2 | 2.25 | 0.70 |
| 2:C:376:PHE:HB2 | 2:C:404:TYR:O | 1.92 | 0.70 |
| 3:CB:202:ARG:HB3 | 3:CB:209:VAL:HG21 | 1.72 | 0.70 |
| 4:CE:10:ILE:HD11 | 4:CE:31:ILE:HD11 | 1.72 | 0.70 |
| 5:CG:290:SER:HB2 | 5:CG:370:HIS:HA | 1.73 | 0.70 |
| 5:CG:491:ASN:HD22 | 5:CG:496:ASP:HB2 | 1.56 | 0.70 |
| 5:CH:305:ASN:HD21 | 5:CH:386:PHE:HB2 | 1.56 | 0.70 |
| 3:D:286:ASN:ND2 | 2:GF:188:ASN:OD1 | 2.23 | 0.70 |
| 1:EB:347:THR:O | 1:EB:350:SER:N | 2.24 | 0.70 |
| 4:G:10:ILE:HD11 | 4:G:31:ILE:HD11 | 1.71 | 0.70 |
| 1:GE:546:ASP:OD1 | 1:GE:547:SER:N | 2.24 | 0.70 |
| 4:GI:84:ARG:HE | 4:HA:64:THR:HA | 1.55 | 0.70 |
| 5:HD:196:ARG:CZ | 7:HI:5:THR:HG23 | 2.21 | 0.70 |
| 7:HH:120:LYS:O | 7:HH:124:ALA:N | 2.24 | 0.70 |
| 7:HI:49:ASP:O | 7:HI:57:ILE:N | 2.22 | 0.70 |
| 5:J:397:ASP:OD1 | 5:J:398:GLU:N | 2.23 | 0.70 |
| 7:P:330:ARG:NH2 | 7:P:336:GLU:OE2 | 2.22 | 0.70 |
| 7:Q:166:GLN:HA | 7:Q:170:ILE:HD12 | 1.74 | 0.70 |
| 7:Q:229:LYS:HG3 | 7:Q:243:VAL:HG12 | 1.73 | 0.70 |
| 7:P:513:ARG:N | 7:Q:441:GLN:O | 2.19 | 0.70 |
| 13:YA:169[D]:ASP:O | 13:YA:272[D]:SER:OG | 2.10 | 0.70 |
| 13:YB:36[A]:PRO:HG3 | 13:YB:45[A]:MET:HB2 | 1.73 | 0.70 |
| 13:YC:57[E]:VAL:HG12 | 13:YC:96[E]:VAL:HB | 1.71 | 0.70 |
| 2:Z:376:PHE:HB2 | 2:Z:404:TYR:O | 1.92 | 0.70 |
| 2:Z:141:THR:HG22 | 2:Z:547:ASN:H | 1.57 | 0.70 |
| 15:ZA:26[D]:GLN:HE22 | 15:ZA:29[D]:VAL:N | 1.85 | 0.70 |
| 5:AC:129:ARG:HG3 | 5:AC:130:PHE:H | 1.57 | 0.70 |
| 1:B:347:THR:O | 1:B:350:SER:N | 2.24 | 0.70 |
| 1:BI:546:ASP:OD1 | 1:BI:547:SER:N | 2.24 | 0.70 |
| 4:CD:168:PHE:HA | 4:CE:163:SER:HB3 | 1.73 | 0.70 |
| 5:CF:406:LEU:O | 5:CH:409:SER:HA | 1.92 | 0.70 |
| 2:EC:199:LEU:HB3 | 2:EC:212:SER:HB2 | 1.72 | 0.70 |
| 2:EC:376:PHE:HB2 | 2:EC:404:TYR:O | 1.92 | 0.70 |
| 2:EC:444:SER:OG | 2:EC:487:MET:SD | 2.49 | 0.70 |
| 2:EC:771:ILE:HD13 | 2:EC:840:ARG:HD3 | 1.71 | 0.70 |
| 3:ED:40:THR:OG1 | 3:ED:273:SER:OG | 2.09 | 0.70 |
| 5:EI:129:ARG:HG3 | 5:EI:130:PHE:H | 1.57 | 0.70 |
| 5:EI:316:ILE:HG23 | 5:EJ:315:GLY:HA3 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:490:TRP:NE1 | 5:EJ:500:ALA:O | 2.23 | 0.70 |
| 2:GF:927:THR:N | 2:GF:985:GLU:OE2 | 2.24 | 0.70 |
| 5:HC:340:VAL:HG23 | 5:HC:341:GLU:HG3 | 1.72 | 0.70 |
| 5:HC:496:ASP:HB3 | 5:HC:500:ALA:HB2 | 1.74 | 0.70 |
| 7:HI:325:TYR:HD1 | 7:HI:330:ARG:HA | 1.57 | 0.70 |
| 7:HI:333:THR:OG1 | 7:HI:335:ASN:OD1 | 2.08 | 0.70 |
| 5:J:98:VAL:HG12 | 5:J:99:PHE:HD2 | 1.56 | 0.70 |
| 5:K:285:LEU:HD11 | 5:K:375:PHE:HB2 | 1.71 | 0.70 |
| 6:M:90:PHE:HD2 | 6:M:126:VAL:HG22 | 1.56 | 0.70 |
| 7:O:193:LEU:HD11 | 7:P:207:GLY:HA2 | 1.73 | 0.70 |
| 7:P:36:ILE:HG21 | 7:Q:18:PHE:HZ | 1.57 | 0.70 |
| 5:I:234:GLN:HE22 | 7:Q:9:VAL:HG21 | 1.57 | 0.70 |
| 8:S:88:TRP:CZ3 | 8:S:134:PRO:HD3 | 2.26 | 0.70 |
| 13:YA:169[B]:ASP:O | 13:YA:272[B]:SER:OG | 2.10 | 0.70 |
| 13:YA:221[F]:LEU:HD12 | 13:YA:229[F]:ILE:HG13 | 1.72 | 0.70 |
| 13:YA:50[A]:GLU:CD | 13:YA:50[A]:GLU:H | 1.91 | 0.70 |
| 13:YA:550[A]:TRP:CD1 | 13:YC:554[A]:MET:HE2 | 2.26 | 0.70 |
| 13:YB:169[A]:ASP:O | 13:YB:272[A]:SER:OG | 2.10 | 0.70 |
| 13:YC:36[D]:PRO:HG3 | 13:YC:45[D]:MET:HB2 | 1.74 | 0.70 |
| 5:AC:406:LEU:O | 5:AE:409:SER:HA | 1.91 | 0.70 |
| 7:AJ:49:ASP:O | 7:AJ:57:ILE:N | 2.22 | 0.70 |
| 8:BC:88:TRP:CZ3 | 8:BC:134:PRO:HD3 | 2.26 | 0.70 |
| 2:BJ:199:LEU:HB3 | 2:BJ:212:SER:HB2 | 1.72 | 0.70 |
| 2:C:138:ASN:O | 2:C:555:ARG:NH1 | 2.25 | 0.70 |
| 2:C:678:GLY:O | 2:C:684:ASN:ND2 | 2.25 | 0.70 |
| 7:DB:120:LYS:O | 7:DB:124:ALA:N | 2.24 | 0.70 |
| 7:DC:496:ARG:NH1 | 7:DC:501:THR:OG1 | 2.24 | 0.70 |
| 8:DE:56:ARG:NH2 | 8:IA:96:GLY:O | 2.24 | 0.70 |
| 5:EI:326:MET:HE1 | 5:EJ:264:ARG:HB3 | 1.73 | 0.70 |
| 1:GE:135:ALA:HA | 1:GE:283:ALA:HA | 1.74 | 0.70 |
| 5:HD:339:GLU:HG2 | 6:HE:173:THR:HB | 1.72 | 0.70 |
| 8:IB:88:TRP:CZ3 | 8:IB:134:PRO:HD3 | 2.27 | 0.70 |
| 1:Y:546:ASP:OD1 | 1:Y:547:SER:N | 2.24 | 0.70 |
| 1:Y:49:GLU:HA | 1:Y:54:ASN:HD22 | 1.57 | 0.70 |
| 13:YA:169[E]:ASP:O | 13:YA:272[E]:SER:OG | 2.10 | 0.70 |
| 13:YA:57[A]:VAL:HG11 | 13:YA:76[A]:PRO:HD3 | 1.72 | 0.70 |
| 2:Z:444:SER:OG | 2:Z:487:MET:SD | 2.49 | 0.70 |
| 1:A:649:GLN:N | 1:A:649:GLN:OE1 | 2.24 | 0.70 |
| 5:AE:305:ASN:HD21 | 5:AE:386:PHE:HB2 | 1.56 | 0.70 |
| 6:AH:90:PHE:HD2 | 6:AH:126:VAL:HG22 | 1.56 | 0.70 |
| 1:BI:553:VAL:N | 1:BI:593:GLY:O | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:DA:90:PHE:HD2 | 6:DA:126:VAL:HG22 | 1.56 | 0.70 |
| 7:DC:100:TYR:OH | 7:DD:113:GLU:O | 2.05 | 0.70 |
| 1:EB:403:PRO:HG3 | 2:EC:885:PRO:HG3 | 1.74 | 0.70 |
| 2:EC:1025:PRO:O | 2:EC:1026:THR:HG22 | 1.92 | 0.70 |
| 2:EC:236:THR:HG22 | 2:EC:515:ASN:HB3 | 1.72 | 0.70 |
| 2:EC:678:GLY:O | 2:EC:684:ASN:ND2 | 2.25 | 0.70 |
| 1:GE:102:SER:H | 1:GE:194:ARG:HH12 | 1.38 | 0.70 |
| 2:GF:303:ASN:OD1 | 2:GF:327:ARG:NH1 | 2.24 | 0.70 |
| 6:HE:90:PHE:HD2 | 6:HE:126:VAL:HG22 | 1.56 | 0.70 |
| 5:I:331:CYS:HA | 5:I:349:TRP:HZ2 | 1.56 | 0.70 |
| 7:P:325:TYR:HD1 | 7:P:330:ARG:HA | 1.57 | 0.70 |
| 1:X:563:VAL:HG22 | 1:X:611:LEU:HD21 | 1.72 | 0.70 |
| 13:YC:169[F]:ASP:O | 13:YC:272[F]:SER:OG | 2.10 | 0.70 |
| 2:Z:138:ASN:O | 2:Z:555:ARG:NH1 | 2.25 | 0.70 |
| 5:AC:331:CYS:HA | 5:AC:349:TRP:HZ2 | 1.56 | 0.70 |
| 1:B:592:ILE:HG12 | 1:B:609:ILE:HD11 | 1.73 | 0.70 |
| 2:BJ:376:PHE:HB2 | 2:BJ:404:TYR:O | 1.92 | 0.70 |
| 2:BJ:411:LYS:HG3 | 2:BJ:412:THR:HG22 | 1.73 | 0.70 |
| 3:D:104:TYR:HB3 | 3:D:166:SER:H | 1.56 | 0.70 |
| 1:EA:466:THR:HG22 | 1:GE:466:THR:HG22 | 1.74 | 0.70 |
| 5:EJ:98:VAL:HG12 | 5:EJ:99:PHE:HD2 | 1.57 | 0.70 |
| 1:GE:23:GLY:H | 11:IE:26:THR:HG1 | 1.39 | 0.70 |
| 2:GF:376:PHE:HB2 | 2:GF:404:TYR:O | 1.92 | 0.70 |
| 6:HF:52:ILE:HD11 | 6:HG:15:ALA:HB2 | 1.74 | 0.70 |
| 5:J:496:ASP:HB3 | 5:J:500:ALA:HB2 | 1.74 | 0.70 |
| 7:P:117:THR:HG23 | 7:P:120:LYS:H | 1.57 | 0.70 |
| 7:O:126:ASN:OD1 | 7:P:132:ARG:NH1 | 2.25 | 0.70 |
| 13:YA:169[C]:ASP:O | 13:YA:272[C]:SER:OG | 2.10 | 0.70 |
| 13:YA:36[A]:PRO:HG3 | 13:YA:45[A]:MET:HB2 | 1.73 | 0.70 |
| 13:YA:57[E]:VAL:HG12 | 13:YA:96[E]:VAL:HB | 1.71 | 0.70 |
| 13:YC:169[D]:ASP:O | 13:YC:272[D]:SER:OG | 2.10 | 0.70 |
| 13:YC:50[C]:GLU:CD | 13:YC:50[C]:GLU:H | 1.91 | 0.70 |
| 13:YB:554[A]:MET:HE2 | 13:YC:550[A]:TRP:CD1 | 2.26 | 0.70 |
| 13:YA:550[B]:TRP:CD1 | 13:YC:554[B]:MET:HE2 | 2.26 | 0.70 |
| 2:Z:199:LEU:HB3 | 2:Z:212:SER:HB2 | 1.72 | 0.70 |
| 2:Z:236:THR:HG22 | 2:Z:515:ASN:HB3 | 1.72 | 0.70 |
| 2:Z:824:GLN:N | 2:Z:837:GLU:OE2 | 2.24 | 0.70 |
| 5:AD:305:ASN:ND2 | 5:AE:255:ARG:O | 2.25 | 0.70 |
| 7:AJ:117:THR:HG23 | 7:AJ:120:LYS:H | 1.57 | 0.70 |
| 7:AJ:12:GLU:HB3 | 7:AJ:15:TYR:HB3 | 1.72 | 0.70 |
| 7:AI:57:ILE:HG22 | 7:AJ:55:LYS:HB3 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:466:THR:HG22 | 1:GD:466:THR:HG22 | 1.74 | 0.70 |
| 1:B:49:GLU:HA | 1:B:54:ASN:HD22 | 1.57 | 0.70 |
| 7:AJ:36:ILE:HG21 | 7:BA:18:PHE:HZ | 1.57 | 0.70 |
| 8:BC:162:TRP:O | 8:DF:95:GLN:NE2 | 2.25 | 0.70 |
| 2:C:411:LYS:HG3 | 2:C:412:THR:HG22 | 1.74 | 0.70 |
| 5:CG:496:ASP:HB3 | 5:CG:500:ALA:HB2 | 1.74 | 0.70 |
| 3:D:40:THR:OG1 | 3:D:273:SER:OG | 2.09 | 0.70 |
| 7:DC:303:GLU:HA | 7:DD:309:ALA:HB3 | 1.74 | 0.70 |
| 7:DC:357:ASP:OD1 | 7:DD:339:ARG:NH2 | 2.25 | 0.70 |
| 3:E:233:GLN:OE1 | 2:GF:529:SER:OG | 2.09 | 0.70 |
| 5:EJ:496:ASP:HB3 | 5:EJ:500:ALA:HB2 | 1.74 | 0.70 |
| 7:FE:486:ASP:HB2 | 7:FF:444:TYR:HB2 | 1.73 | 0.70 |
| 7:FF:513:ARG:N | 7:FG:441:GLN:O | 2.18 | 0.70 |
| 5:HC:507:ASP:OD1 | 5:HC:511:ASN:N | 2.22 | 0.70 |
| 5:HC:98:VAL:HG12 | 5:HC:99:PHE:HD2 | 1.57 | 0.70 |
| 5:HB:196:ARG:NH2 | 5:HD:199:GLU:OE1 | 2.24 | 0.70 |
| 5:I:84:GLY:O | 5:I:86:VAL:N | 2.22 | 0.70 |
| 5:J:340:VAL:HG23 | 5:J:341:GLU:HG3 | 1.72 | 0.70 |
| 5:I:406:LEU:O | 5:K:409:SER:HA | 1.92 | 0.70 |
| 7:O:69:GLY:HA2 | 7:Q:78:PRO:HB2 | 1.73 | 0.70 |
| 8:R:88:TRP:CZ3 | 8:R:134:PRO:HD3 | 2.26 | 0.70 |
| 13:YB:321[F]:LYS:HD3 | 13:YC:452[F]:GLY:HA2 | 1.74 | 0.70 |
| 13:YB:468[A]:ASP:OD2 | 13:YC:461[A]:SER:OG | 2.10 | 0.70 |
| 2:Z:303:ASN:OD1 | 2:Z:327:ARG:NH1 | 2.24 | 0.70 |
| 1:A:466:THR:HG22 | 1:Y:466:THR:HG22 | 1.74 | 0.69 |
| 5:AC:316:ILE:HG23 | 5:AD:315:GLY:HA3 | 1.74 | 0.69 |
| 7:AJ:366:THR:HG22 | 7:AJ:391:GLY:HA2 | 1.72 | 0.69 |
| 1:B:240:GLU:OE1 | 1:B:240:GLU:N | 2.22 | 0.69 |
| 8:BB:88:TRP:CZ3 | 8:BB:134:PRO:HD3 | 2.26 | 0.69 |
| 2:BJ:67:PHE:CE2 | 2:BJ:69:PHE:HB2 | 2.27 | 0.69 |
| 3:D:115:ASN:OD1 | 3:D:122:THR:N | 2.25 | 0.69 |
| 7:DB:401:ARG:HB3 | 7:DD:399:PHE:HE1 | 1.54 | 0.69 |
| 1:EB:135:ALA:HA | 1:EB:283:ALA:HA | 1.74 | 0.69 |
| 1:EB:592:ILE:HG12 | 1:EB:609:ILE:HD11 | 1.73 | 0.69 |
| 2:EC:991:SER:O | 2:EC:993:LEU:N | 2.24 | 0.69 |
| 5:EJ:339:GLU:HB2 | 6:FD:171:TYR:HB2 | 1.73 | 0.69 |
| 7:FE:188:GLN:HG3 | 7:FG:192:GLN:HB2 | 1.74 | 0.69 |
| 7:FE:199:VAL:HA | 7:FG:212:PRO:HB3 | 1.73 | 0.69 |
| 2:GF:67:PHE:CE2 | 2:GF:69:PHE:HB2 | 2.27 | 0.69 |
| 5:HC:34:TYR:OH | 5:HC:40:GLY:O | 2.03 | 0.69 |
| 7:HH:199:VAL:HA | 7:HJ:212:PRO:HB3 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:196:ARG:NH2 | 7:HJ:9:VAL:HG12 | 2.06 | 0.69 |
| 2:GF:664:PHE:HB2 | 9:IC:15:MET:HB2 | 1.72 | 0.69 |
| 1:Y:135:ALA:HA | 1:Y:283:ALA:HA | 1.74 | 0.69 |
| 1:Y:403:PRO:HG3 | 2:Z:885:PRO:HG3 | 1.74 | 0.69 |
| 1:Y:553:VAL:N | 1:Y:593:GLY:O | 2.23 | 0.69 |
| 13:YA:405[B]:ASP:OD1 | 13:YC:397[B]:SER:OG | 2.10 | 0.69 |
| 13:YB:169[F]:ASP:O | 13:YB:272[F]:SER:OG | 2.10 | 0.69 |
| 13:YC:169[A]:ASP:O | 13:YC:272[A]:SER:OG | 2.10 | 0.69 |
| 2:Z:1025:PRO:O | 2:Z:1026:THR:HG22 | 1.92 | 0.69 |
| 2:BJ:991:SER:O | 2:BJ:993:LEU:N | 2.24 | 0.69 |
| 2:C:141:THR:HG22 | 2:C:547:ASN:H | 1.57 | 0.69 |
| 8:DE:88:TRP:CZ3 | 8:DE:134:PRO:HD3 | 2.26 | 0.69 |
| 5:EJ:491:ASN:HD22 | 5:EJ:496:ASP:HB2 | 1.56 | 0.69 |
| 7:FF:496:ARG:NH1 | 7:FF:501:THR:OG1 | 2.24 | 0.69 |
| 7:HI:117:THR:HG23 | 7:HI:120:LYS:H | 1.57 | 0.69 |
| 5:K:305:ASN:HD21 | 5:K:386:PHE:HB2 | 1.56 | 0.69 |
| 6:M:70:ILE:HG12 | 6:N:73:ASN:HA | 1.75 | 0.69 |
| 7:O:486:ASP:HB2 | 7:P:444:TYR:HB2 | 1.72 | 0.69 |
| 7:P:496:ARG:NH1 | 7:P:501:THR:OG1 | 2.24 | 0.69 |
| 13:YB:221[C]:LEU:HD12 | 13:YB:229[C]:ILE:HG13 | 1.72 | 0.69 |
| 13:YB:36[B]:PRO:HG3 | 13:YB:45[B]:MET:HB2 | 1.73 | 0.69 |
| 2:Z:678:GLY:O | 2:Z:684:ASN:ND2 | 2.25 | 0.69 |
| 5:AD:496:ASP:HB3 | 5:AD:500:ALA:HB2 | 1.74 | 0.69 |
| 7:AJ:50:ALA:HA | 7:AJ:56:GLY:HA3 | 1.74 | 0.69 |
| 1:B:135:ALA:HA | 1:B:283:ALA:HA | 1.74 | 0.69 |
| 3:CA:115:ASN:OD1 | 3:CA:122:THR:N | 2.25 | 0.69 |
| 7:DB:486:ASP:HB2 | 7:DC:444:TYR:HB2 | 1.74 | 0.69 |
| 1:EB:23:GLY:H | 11:GB:26:THR:HG1 | 1.40 | 0.69 |
| 2:EC:968:ASP:HB3 | 2:EC:972:GLU:HG2 | 1.73 | 0.69 |
| 7:FE:69:GLY:HA2 | 7:FG:78:PRO:HB2 | 1.75 | 0.69 |
| 8:FH:88:TRP:CZ3 | 8:FH:134:PRO:HD3 | 2.26 | 0.69 |
| 1:GE:403:PRO:HG3 | 2:GF:885:PRO:HG3 | 1.74 | 0.69 |
| 2:GF:138:ASN:O | 2:GF:555:ARG:NH1 | 2.25 | 0.69 |
| 2:GF:968:ASP:HB3 | 2:GF:972:GLU:HG2 | 1.73 | 0.69 |
| 5:HB:144:GLU:HB3 | 5:HC:151:ILE:HD13 | 1.75 | 0.69 |
| 5:HB:312:ARG:HG2 | 5:HB:317:LEU:HA | 1.73 | 0.69 |
| 7:HH:69:GLY:HA2 | 7:HJ:78:PRO:HB2 | 1.75 | 0.69 |
| 7:O:448:ALA:N | 7:P:485:ASN:OD1 | 2.25 | 0.69 |
| 7:P:40:SER:HB3 | 7:Q:24:ASN:HB2 | 1.73 | 0.69 |
| 1:Y:592:ILE:HG12 | 1:Y:609:ILE:HD11 | 1.73 | 0.69 |
| 13:YB:169[E]:ASP:O | 13:YB:272[E]:SER:OG | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:468[C]:ASP:OD2 | 13:YC:461[C]:SER:OG | 2.11 | 0.69 |
| 13:YC:81[E]:ARG:NH2 | 13:YC:101[E]:GLY:HA2 | 2.07 | 0.69 |
| 14:YD:36[C]:THR:HG22 | 14:YD:37[C]:THR:HG23 | 1.74 | 0.69 |
| 14:YF:211[E]:MET:HE1 | 14:YF:231[E]:ALA:HB2 | 1.74 | 0.69 |
| 6:AF:90:PHE:HD2 | 6:AF:126:VAL:HG22 | 1.56 | 0.69 |
| 2:C:1025:PRO:O | 2:C:1026:THR:HG22 | 1.92 | 0.69 |
| 7:DC:117:THR:HG23 | 7:DC:120:LYS:H | 1.57 | 0.69 |
| 7:DC:12:GLU:HB3 | 7:DC:15:TYR:HB3 | 1.72 | 0.69 |
| 8:DF:88:TRP:CZ3 | 8:DF:134:PRO:HD3 | 2.26 | 0.69 |
| 1:EA:127:ARG:N | 1:EA:150:ASP:OD1 | 2.26 | 0.69 |
| 1:EA:517:PHE:N | 1:EA:536:TYR:O | 2.24 | 0.69 |
| 1:EB:546:ASP:OD1 | 1:EB:547:SER:N | 2.24 | 0.69 |
| 5:EJ:326:MET:HE3 | 5:FA:279:SER:HA | 1.74 | 0.69 |
| 6:FC:90:PHE:HD2 | 6:FC:126:VAL:HG22 | 1.56 | 0.69 |
| 1:GD:195:ASN:OD1 | 1:GD:352:ARG:NH1 | 2.23 | 0.69 |
| 2:GF:374:LYS:NZ | 2:GF:499:GLU:OE2 | 2.18 | 0.69 |
| 6:HF:90:PHE:HD2 | 6:HF:126:VAL:HG22 | 1.56 | 0.69 |
| 6:HG:90:PHE:HD2 | 6:HG:126:VAL:HG22 | 1.56 | 0.69 |
| 10:ID:129:LEU:HD13 | 10:ID:209:TRP:CZ3 | 2.28 | 0.69 |
| 5:J:391:GLY:HA3 | 5:K:390:LEU:HD13 | 1.74 | 0.69 |
| 13:YA:50[E]:GLU:CD | 13:YA:50[E]:GLU:H | 1.91 | 0.69 |
| 13:YC:169[B]:ASP:O | 13:YC:272[B]:SER:OG | 2.10 | 0.69 |
| 13:YC:50[A]:GLU:CD | 13:YC:50[A]:GLU:H | 1.91 | 0.69 |
| 1:Y:338:ARG:NH1 | 2:Z:738:LYS:O | 2.22 | 0.69 |
| 1:A:215:VAL:HG21 | 1:A:252:LEU:HD13 | 1.75 | 0.69 |
| 5:AD:491:ASN:HD22 | 5:AD:496:ASP:HB2 | 1.56 | 0.69 |
| 5:CG:311:VAL:HG11 | 5:CG:321:ALA:H | 1.58 | 0.69 |
| 7:DD:166:GLN:HA | 7:DD:170:ILE:HD12 | 1.74 | 0.69 |
| 2:EC:927:THR:N | 2:EC:985:GLU:OE2 | 2.24 | 0.69 |
| 7:FF:36:ILE:HG21 | 7:FG:18:PHE:HZ | 1.57 | 0.69 |
| 1:GD:127:ARG:N | 1:GD:150:ASP:OD1 | 2.26 | 0.69 |
| 2:GF:411:LYS:HG3 | 2:GF:412:THR:HG22 | 1.73 | 0.69 |
| 2:GF:678:GLY:O | 2:GF:684:ASN:ND2 | 2.25 | 0.69 |
| 5:HC:491:ASN:HD22 | 5:HC:496:ASP:HB2 | 1.56 | 0.69 |
| 7:HH:193:LEU:HD11 | 7:HI:207:GLY:HA2 | 1.73 | 0.69 |
| 7:HH:366:THR:HG22 | 7:HH:391:GLY:HA2 | 1.73 | 0.69 |
| 1:X:195:ASN:OD1 | 1:X:352:ARG:NH1 | 2.24 | 0.69 |
| 13:YB:112[E]:GLU:HA | 13:YB:113[E]:GLY:N | 2.07 | 0.69 |
| 13:YB:169[C]:ASP:O | 13:YB:272[C]:SER:OG | 2.10 | 0.69 |
| 14:YF:184[C]:LYS:NZ | 14:YF:201[C]:ASP:OD2 | 2.26 | 0.69 |
| 2:Z:241:SER:OG | 2:Z:315:ASP:OD1 | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:40:SER:HB3 | 7:BA:24:ASN:HB2 | 1.73 | 0.69 |
| 1:A:63:ASN:ND2 | 1:B:60:LEU:HB3 | 2.08 | 0.69 |
| 1:BI:135:ALA:HA | 1:BI:283:ALA:HA | 1.74 | 0.69 |
| 2:BJ:932:ARG:HG3 | 2:BJ:1005:ARG:NH2 | 2.08 | 0.69 |
| 1:BI:230:ILE:HD13 | 2:BJ:691:ARG:HG3 | 1.74 | 0.69 |
| 2:BJ:968:ASP:HB3 | 2:BJ:972:GLU:HG2 | 1.73 | 0.69 |
| 2:BJ:927:THR:N | 2:BJ:985:GLU:OE2 | 2.24 | 0.69 |
| 2:C:241:SER:OG | 2:C:315:ASP:OD1 | 2.10 | 0.69 |
| 2:C:968:ASP:HB3 | 2:C:972:GLU:HG2 | 1.73 | 0.69 |
| 3:CA:40:THR:OG1 | 3:CA:273:SER:OG | 2.09 | 0.69 |
| 5:CG:98:VAL:HG12 | 5:CG:99:PHE:HD2 | 1.57 | 0.69 |
| 5:FA:323:THR:HG23 | 5:FA:359:GLU:HB2 | 1.74 | 0.69 |
| 7:FE:193:LEU:HD11 | 7:FF:207:GLY:HA2 | 1.73 | 0.69 |
| 2:GF:141:THR:HG22 | 2:GF:547:ASN:H | 1.57 | 0.69 |
| 4:GI:122:LEU:HB3 | 4:GI:139:VAL:HB | 1.75 | 0.69 |
| 4:F:103:LEU:HD21 | 4:H:113:ASN:HD22 | 1.58 | 0.69 |
| 7:HI:357:ASP:OD1 | 7:HJ:339:ARG:NH2 | 2.25 | 0.69 |
| 1:Y:612:THR:HG22 | 1:Y:614:GLU:H | 1.58 | 0.69 |
| 13:YA:169[A]:ASP:O | 13:YA:272[A]:SER:OG | 2.10 | 0.69 |
| 13:YB:112[D]:GLU:HA | 13:YB:113[D]:GLY:N | 2.07 | 0.69 |
| 13:YB:321[C]:LYS:HD3 | 13:YC:452[C]:GLY:HA2 | 1.73 | 0.69 |
| 13:YB:36[F]:PRO:HG3 | 13:YB:45[F]:MET:HB2 | 1.75 | 0.69 |
| 13:YB:468[D]:ASP:OD2 | 13:YC:461[D]:SER:OG | 2.10 | 0.69 |
| 13:YB:468[F]:ASP:OD2 | 13:YC:461[F]:SER:OG | 2.11 | 0.69 |
| 14:YD:17[A]:PHE:CD2 | 14:YD:23[A]:TRP:HA | 2.27 | 0.69 |
| 14:YF:36[E]:THR:HG22 | 14:YF:37[E]:THR:HG23 | 1.75 | 0.69 |
| 2:BJ:138:ASN:O | 2:BJ:555:ARG:NH1 | 2.25 | 0.69 |
| 2:BJ:174:HIS:ND1 | 2:BJ:508:TYR:OH | 2.26 | 0.69 |
| 2:BJ:174:HIS:NE2 | 3:EE:227:ASP:OD2 | 2.26 | 0.69 |
| 2:BJ:824:GLN:N | 2:BJ:837:GLU:OE2 | 2.24 | 0.69 |
| 5:CG:265:LEU:HB3 | 5:CG:281:TYR:HB3 | 1.75 | 0.69 |
| 1:EA:215:VAL:HG21 | 1:EA:252:LEU:HD13 | 1.75 | 0.69 |
| 2:EC:932:ARG:HG3 | 2:EC:1005:ARG:NH2 | 2.08 | 0.69 |
| 2:EC:67:PHE:CE2 | 2:EC:69:PHE:HB2 | 2.27 | 0.69 |
| 4:EG:122:LEU:HB3 | 4:EG:139:VAL:HB | 1.75 | 0.69 |
| 5:EJ:196:ARG:NH2 | 7:FG:9:VAL:HG12 | 2.07 | 0.69 |
| 4:F:122:LEU:HB3 | 4:F:139:VAL:HB | 1.75 | 0.69 |
| 2:GF:433:ASN:OD1 | 2:GF:434:MET:N | 2.25 | 0.69 |
| 5:HB:326:MET:HE1 | 5:HC:264:ARG:HB3 | 1.74 | 0.69 |
| 5:HB:251:VAL:HG11 | 5:HD:254:TRP:CZ2 | 2.27 | 0.69 |
| 7:HH:126:ASN:OD1 | 7:HI:132:ARG:NH1 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:36:ILE:HG21 | 7:HJ:18:PHE:HZ | 1.58 | 0.69 |
| 5:J:34:TYR:OH | 5:J:40:GLY:O | 2.03 | 0.69 |
| 1:B:76:TYR:OH | 11:V:29:PHE:O | 2.09 | 0.69 |
| 12:W:216:PHE:HE1 | 12:W:218:MET:HE3 | 1.57 | 0.69 |
| 13:YA:112[F]:GLU:HA | 13:YA:113[F]:GLY:N | 2.07 | 0.69 |
| 13:YB:558[B]:SER:HB3 | 13:YC:551[B]:THR:HG22 | 1.75 | 0.69 |
| 13:YC:112[C]:GLU:HA | 13:YC:113[C]:GLY:N | 2.07 | 0.69 |
| 13:YC:36[B]:PRO:HG3 | 13:YC:45[B]:MET:HB2 | 1.73 | 0.69 |
| 13:YA:550[D]:TRP:CD1 | 13:YC:554[D]:MET:HE2 | 2.28 | 0.69 |
| 14:YD:184[A]:LYS:NZ | 14:YD:201[A]:ASP:OD2 | 2.26 | 0.69 |
| 14:YD:36[B]:THR:HG22 | 14:YD:37[B]:THR:HG23 | 1.74 | 0.69 |
| 14:YE:184[E]:LYS:NZ | 14:YE:201[E]:ASP:OD2 | 2.26 | 0.69 |
| 5:AE:323:THR:HG23 | 5:AE:359:GLU:HB2 | 1.74 | 0.69 |
| 7:AJ:496:ARG:NH1 | 7:AJ:501:THR:OG1 | 2.24 | 0.69 |
| 1:B:403:PRO:HG3 | 2:C:885:PRO:HG3 | 1.74 | 0.69 |
| 1:B:619:GLN:HG2 | 1:B:620:THR:HG23 | 1.75 | 0.69 |
| 1:BI:592:ILE:HG12 | 1:BI:609:ILE:HD11 | 1.73 | 0.69 |
| 1:BI:612:THR:HG22 | 1:BI:614:GLU:H | 1.58 | 0.69 |
| 2:C:1000:THR:HA | 5:I:18:TYR:HA | 1.75 | 0.69 |
| 2:C:932:ARG:HG3 | 2:C:1005:ARG:NH2 | 2.08 | 0.69 |
| 2:C:233:LEU:HD12 | 2:C:391:ARG:HB2 | 1.75 | 0.69 |
| 5:CF:331:CYS:HA | 5:CF:349:TRP:HZ2 | 1.56 | 0.69 |
| 6:CJ:90:PHE:HD2 | 6:CJ:126:VAL:HG22 | 1.56 | 0.69 |
| 7:DC:40:SER:HB3 | 7:DD:24:ASN:HB2 | 1.72 | 0.69 |
| 10:DH:129:LEU:HD13 | 10:DH:209:TRP:CZ3 | 2.28 | 0.69 |
| 1:EB:174:ARG:HH21 | 1:EB:269:VAL:HG21 | 1.58 | 0.69 |
| 1:EB:76:TYR:OH | 11:GB:29:PHE:O | 2.11 | 0.69 |
| 4:EF:113:ASN:HD22 | 4:EG:103:LEU:HD21 | 1.56 | 0.69 |
| 5:EJ:594:THR:HB | 5:FA:490:TRP:HB2 | 1.75 | 0.69 |
| 7:FE:366:THR:HG22 | 7:FE:391:GLY:HA2 | 1.73 | 0.69 |
| 7:FF:325:TYR:HD1 | 7:FF:330:ARG:HA | 1.57 | 0.69 |
| 1:GE:592:ILE:HG12 | 1:GE:609:ILE:HD11 | 1.73 | 0.69 |
| 2:GF:241:SER:OG | 2:GF:315:ASP:OD1 | 2.10 | 0.69 |
| 7:O:366:THR:HG22 | 7:O:391:GLY:HA2 | 1.73 | 0.69 |
| 1:Y:619:GLN:HG2 | 1:Y:620:THR:HG23 | 1.75 | 0.69 |
| 13:YA:405[C]:ASP:OD1 | 13:YC:397[C]:SER:OG | 2.11 | 0.69 |
| 13:YB:321[D]:LYS:HD3 | 13:YC:452[D]:GLY:HA2 | 1.74 | 0.69 |
| 13:YB:558[C]:SER:HB3 | 13:YC:551[C]:THR:HG22 | 1.75 | 0.69 |
| 13:YC:112[B]:GLU:HA | 13:YC:113[B]:GLY:N | 2.07 | 0.69 |
| 11:V:190:LYS:HE3 | 14:YD:24[B]:SER:O | 1.90 | 0.69 |
| 14:YE:17[B]:PHE:CD2 | 14:YE:23[B]:TRP:HA | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:36[B]:THR:HG22 | 14:YE:37[B]:THR:HG23 | 1.74 | 0.69 |
| 14:YF:17[C]:PHE:CD2 | 14:YF:23[C]:TRP:HA | 2.27 | 0.69 |
| 2:Z:174:HIS:ND1 | 2:Z:508:TYR:OH | 2.26 | 0.69 |
| 5:AD:98:VAL:HG12 | 5:AD:99:PHE:HD2 | 1.57 | 0.69 |
| 6:AF:58:ASP:OD1 | 6:AG:164:GLN:NE2 | 2.25 | 0.69 |
| 7:BA:166:GLN:HA | 7:BA:170:ILE:HD12 | 1.74 | 0.69 |
| 12:BG:24:CYS:HB3 | 12:BG:125:ILE:HG21 | 1.75 | 0.69 |
| 1:BI:243:ILE:HD11 | 1:BI:252:LEU:HB3 | 1.75 | 0.69 |
| 2:BJ:433:ASN:OD1 | 2:BJ:434:MET:N | 2.25 | 0.69 |
| 7:DC:71:ASN:HB2 | 7:FG:365:GLY:HA2 | 1.74 | 0.69 |
| 1:EA:63:ASN:ND2 | 1:EB:60:LEU:HB3 | 2.08 | 0.69 |
| 1:EB:139:SER:OG | 1:EB:141:ASN:OD1 | 2.04 | 0.69 |
| 2:EC:824:GLN:N | 2:EC:837:GLU:OE2 | 2.24 | 0.69 |
| 3:ED:115:ASN:OD1 | 3:ED:122:THR:N | 2.25 | 0.69 |
| 3:EE:260:GLU:OE1 | 3:EE:260:GLU:N | 2.21 | 0.69 |
| 5:EJ:594:THR:OG1 | 5:FA:517:GLY:N | 2.25 | 0.69 |
| 7:FG:166:GLN:HA | 7:FG:170:ILE:HD12 | 1.74 | 0.69 |
| 1:GD:215:VAL:HG21 | 1:GD:252:LEU:HD13 | 1.75 | 0.69 |
| 2:GF:1025:PRO:O | 2:GF:1026:THR:HG22 | 1.92 | 0.69 |
| 2:GF:233:LEU:HD12 | 2:GF:391:ARG:HB2 | 1.75 | 0.69 |
| 4:GJ:122:LEU:HB3 | 4:GJ:139:VAL:HB | 1.75 | 0.69 |
| 7:HI:197:ALA:O | 7:HI:201:GLN:HG3 | 1.93 | 0.69 |
| 5:I:312:ARG:HG2 | 5:I:317:LEU:HA | 1.73 | 0.69 |
| 8:R:138:GLY:HA3 | 8:IA:43:ALA:HB1 | 1.73 | 0.69 |
| 6:L:90:PHE:HD2 | 6:L:126:VAL:HG22 | 1.56 | 0.69 |
| 7:P:333:THR:OG1 | 7:P:335:ASN:OD1 | 2.08 | 0.69 |
| 7:P:357:ASP:OD1 | 7:Q:339:ARG:NH2 | 2.25 | 0.69 |
| 10:U:129:LEU:HD13 | 10:U:209:TRP:CZ3 | 2.28 | 0.69 |
| 1:Y:174:ARG:HH21 | 1:Y:269:VAL:HG21 | 1.58 | 0.69 |
| 13:YA:112[A]:GLU:HA | 13:YA:113[A]:GLY:N | 2.07 | 0.69 |
| 13:YA:405[A]:ASP:OD1 | 13:YC:397[A]:SER:OG | 2.11 | 0.69 |
| 13:YB:169[D]:ASP:O | 13:YB:272[D]:SER:OG | 2.10 | 0.69 |
| 13:YC:169[C]:ASP:O | 13:YC:272[C]:SER:OG | 2.10 | 0.69 |
| 14:YE:184[C]:LYS:NZ | 14:YE:201[C]:ASP:OD2 | 2.26 | 0.69 |
| 14:YE:36[F]:THR:HG22 | 14:YE:37[F]:THR:HG23 | 1.74 | 0.69 |
| 2:Z:67:PHE:CE2 | 2:Z:69:PHE:HB2 | 2.27 | 0.69 |
| 5:AD:311:VAL:HG11 | 5:AD:321:ALA:H | 1.58 | 0.69 |
| 6:AG:90:PHE:HD2 | 6:AG:126:VAL:HG22 | 1.56 | 0.69 |
| 7:AI:69:GLY:HA2 | 7:BA:78:PRO:HB2 | 1.75 | 0.69 |
| 7:AI:126:ASN:OD1 | 7:AJ:132:ARG:NH1 | 2.25 | 0.69 |
| 2:BJ:188:ASN:OD1 | 3:ED:286:ASN:ND2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:344:THR:OG1 | 2:C:347:GLU:OE1 | 2.09 | 0.69 |
| 2:C:927:THR:N | 2:C:985:GLU:OE2 | 2.24 | 0.69 |
| 3:CA:104:TYR:HB3 | 3:CA:166:SER:H | 1.56 | 0.69 |
| 4:CD:122:LEU:HB3 | 4:CD:139:VAL:HB | 1.75 | 0.69 |
| 5:CF:129:ARG:HG3 | 5:CF:130:PHE:H | 1.57 | 0.69 |
| 5:CF:200:LEU:HB2 | 7:DD:5:THR:HG21 | 1.75 | 0.69 |
| 5:CF:501:LEU:HB3 | 5:CF:512:PRO:HB2 | 1.74 | 0.69 |
| 6:CJ:70:ILE:HG12 | 6:DA:73:ASN:HA | 1.74 | 0.69 |
| 8:DF:162:TRP:O | 8:FI:95:GLN:NE2 | 2.24 | 0.69 |
| 1:EA:195:ASN:OD1 | 1:EA:352:ARG:NH1 | 2.24 | 0.69 |
| 8:FI:88:TRP:CZ3 | 8:FI:134:PRO:HD3 | 2.26 | 0.69 |
| 1:GE:361:GLN:OE1 | 1:GE:362:THR:N | 2.23 | 0.69 |
| 1:GE:49:GLU:HA | 1:GE:54:ASN:HD22 | 1.57 | 0.69 |
| 3:GG:115:ASN:OD1 | 3:GG:122:THR:N | 2.25 | 0.69 |
| 5:HB:312:ARG:O | 5:HB:382:ASN:N | 2.25 | 0.69 |
| 5:HB:331:CYS:HA | 5:HB:349:TRP:HZ2 | 1.56 | 0.69 |
| 5:I:129:ARG:HG3 | 5:I:130:PHE:H | 1.57 | 0.69 |
| 7:P:197:ALA:O | 7:P:201:GLN:HG3 | 1.93 | 0.69 |
| 7:O:220:SER:OG | 7:Q:228:ILE:O | 2.05 | 0.69 |
| 1:X:127:ARG:N | 1:X:150:ASP:OD1 | 2.26 | 0.69 |
| 1:X:649:GLN:N | 1:X:649:GLN:OE1 | 2.25 | 0.69 |
| 1:X:66:TYR:CE1 | 1:Y:21:PHE:HB2 | 2.26 | 0.69 |
| 13:YA:169[F]:ASP:O | 13:YA:272[F]:SER:OG | 2.10 | 0.69 |
| 13:YA:550[C]:TRP:CD1 | 13:YC:554[C]:MET:HE2 | 2.28 | 0.69 |
| 13:YB:112[F]:GLU:HA | 13:YB:113[F]:GLY:N | 2.07 | 0.69 |
| 13:YB:558[D]:SER:HB3 | 13:YC:551[D]:THR:HG22 | 1.75 | 0.69 |
| 14:YD:184[D]:LYS:NZ | 14:YD:201[D]:ASP:OD2 | 2.26 | 0.69 |
| 14:YF:17[F]:PHE:CD2 | 14:YF:23[F]:TRP:HA | 2.28 | 0.69 |
| 14:YF:36[F]:THR:HG22 | 14:YF:37[F]:THR:HG23 | 1.74 | 0.69 |
| 2:Z:433:ASN:OD1 | 2:Z:434:MET:N | 2.25 | 0.69 |
| 5:AC:501:LEU:HB3 | 5:AC:512:PRO:HB2 | 1.74 | 0.69 |
| 5:AD:194:LYS:O | 5:AD:242:VAL:HA | 1.93 | 0.69 |
| 1:BH:466:THR:HG22 | 1:EB:466:THR:HG22 | 1.74 | 0.69 |
| 2:C:67:PHE:CE2 | 2:C:69:PHE:HB2 | 2.27 | 0.69 |
| 5:CG:344:VAL:HG12 | 5:CG:349:TRP:H | 1.58 | 0.69 |
| 7:DC:330:ARG:NH2 | 7:DC:336:GLU:OE2 | 2.22 | 0.69 |
| 2:EC:138:ASN:O | 2:EC:555:ARG:NH1 | 2.25 | 0.69 |
| 5:EI:144:GLU:HB3 | 5:EJ:151:ILE:HD13 | 1.75 | 0.69 |
| 5:EI:501:LEU:HB3 | 5:EI:512:PRO:HB2 | 1.74 | 0.69 |
| 5:EJ:194:LYS:O | 5:EJ:242:VAL:HA | 1.93 | 0.69 |
| 7:FE:126:ASN:OD1 | 7:FF:132:ARG:NH1 | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:361:ASP:HB3 | 7:FE:472:ARG:NH2 | 2.09 | 0.69 |
| 7:FF:303:GLU:HA | 7:FG:309:ALA:HB3 | 1.74 | 0.69 |
| 2:GF:251:ASP:OD2 | 2:GF:252:LYS:NZ | 2.26 | 0.69 |
| 2:GF:344:THR:OG1 | 2:GF:347:GLU:OE1 | 2.09 | 0.69 |
| 3:GG:40:THR:OG1 | 3:GG:273:SER:OG | 2.09 | 0.69 |
| 5:HB:129:ARG:HG3 | 5:HB:130:PHE:H | 1.57 | 0.69 |
| 5:HD:323:THR:HG23 | 5:HD:359:GLU:HB2 | 1.74 | 0.69 |
| 7:HI:303:GLU:HA | 7:HJ:309:ALA:HB3 | 1.75 | 0.69 |
| 5:J:265:LEU:HB3 | 5:J:281:TYR:HB3 | 1.75 | 0.69 |
| 7:P:303:GLU:HA | 7:Q:309:ALA:HB3 | 1.74 | 0.69 |
| 12:W:24:CYS:HB3 | 12:W:125:ILE:HG21 | 1.75 | 0.69 |
| 13:YA:36[C]:PRO:HG3 | 13:YA:45[C]:MET:HB2 | 1.75 | 0.69 |
| 13:YA:405[F]:ASP:OD1 | 13:YC:397[F]:SER:OG | 2.11 | 0.69 |
| 14:YD:184[C]:LYS:NZ | 14:YD:201[C]:ASP:OD2 | 2.26 | 0.69 |
| 14:YD:17[B]:PHE:CD2 | 14:YD:23[B]:TRP:HA | 2.28 | 0.69 |
| 14:YF:17[A]:PHE:CD2 | 14:YF:23[A]:TRP:HA | 2.27 | 0.69 |
| 14:YF:184[A]:LYS:NZ | 14:YF:201[A]:ASP:OD2 | 2.26 | 0.69 |
| 14:YF:184[D]:LYS:NZ | 14:YF:201[D]:ASP:OD2 | 2.26 | 0.69 |
| 10:BE:129:LEU:HD13 | 10:BE:209:TRP:CZ3 | 2.28 | 0.68 |
| 2:C:214:ASP:HB2 | 2:C:217:GLN:HE22 | 1.58 | 0.68 |
| 2:C:3:VAL:O | 2:C:90:GLU:N | 2.26 | 0.68 |
| 7:DB:447:HIS:HD2 | 7:DC:447:HIS:CD2 | 2.11 | 0.68 |
| 7:DC:197:ALA:O | 7:DC:201:GLN:HG3 | 1.93 | 0.68 |
| 2:EC:411:LYS:HG3 | 2:EC:412:THR:HG22 | 1.73 | 0.68 |
| 2:EC:141:THR:HG22 | 2:EC:547:ASN:H | 1.57 | 0.68 |
| 5:FA:194:LYS:HB2 | 5:FA:243:GLN:HB2 | 1.75 | 0.68 |
| 7:FF:197:ALA:O | 7:FF:201:GLN:HG3 | 1.93 | 0.68 |
| 10:GA:129:LEU:HD13 | 10:GA:209:TRP:CZ3 | 2.28 | 0.68 |
| 2:GF:444:SER:OG | 2:GF:487:MET:SD | 2.49 | 0.68 |
| 2:GF:824:GLN:N | 2:GF:837:GLU:OE2 | 2.24 | 0.68 |
| 5:HC:311:VAL:HG11 | 5:HC:321:ALA:H | 1.58 | 0.68 |
| 7:HH:57:ILE:HG22 | 7:HI:55:LYS:HB3 | 1.74 | 0.68 |
| 7:P:96:GLY:O | 8:IB:56:ARG:NH2 | 353.96 | 0.68 |
| 13:YA:36[E]:PRO:HG3 | 13:YA:45[E]:MET:HB2 | 1.73 | 0.68 |
| 13:YB:558[E]:SER:HB3 | 13:YC:551[E]:THR:HG22 | 1.74 | 0.68 |
| 14:YD:184[E]:LYS:NZ | 14:YD:201[E]:ASP:OD2 | 2.26 | 0.68 |
| 14:YE:17[E]:PHE:CD2 | 14:YE:23[E]:TRP:HA | 2.27 | 0.68 |
| 14:YE:184[A]:LYS:NZ | 14:YE:201[A]:ASP:OD2 | 2.26 | 0.68 |
| 14:YE:184[B]:LYS:NZ | 14:YE:201[B]:ASP:OD2 | 2.26 | 0.68 |
| 14:YE:211[C]:MET:HE1 | 14:YE:231[C]:ALA:HB2 | 1.74 | 0.68 |
| 14:YE:17[C]:PHE:CD2 | 14:YE:23[C]:TRP:HA | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:184[F]:LYS:NZ | 14:YF:201[F]:ASP:OD2 | 2.26 | 0.68 |
| 14:YF:36[A]:THR:HG22 | 14:YF:37[A]:THR:HG23 | 1.73 | 0.68 |
| 7:AJ:357:ASP:OD1 | 7:BA:339:ARG:NH2 | 2.25 | 0.68 |
| 1:B:38:ASN:ND2 | 1:X:264:GLN:OE1 | 2.26 | 0.68 |
| 1:BI:358:GLN:HB2 | 1:BI:379:LYS:HB3 | 1.76 | 0.68 |
| 2:BJ:332:SER:OG | 2:BJ:333:ASN:O | 2.11 | 0.68 |
| 2:BJ:3:VAL:O | 2:BJ:90:GLU:N | 2.26 | 0.68 |
| 5:CF:144:GLU:HB3 | 5:CG:151:ILE:HD13 | 1.75 | 0.68 |
| 5:CH:353:HIS:CD2 | 7:HJ:476:ASP:HB2 | 2.28 | 0.68 |
| 8:DF:56:ARG:NH2 | 8:IB:96:GLY:O | 2.26 | 0.68 |
| 2:EC:214:ASP:HB2 | 2:EC:217:GLN:HE22 | 1.58 | 0.68 |
| 3:ED:282:LYS:NZ | 3:ED:289:ASN:OD1 | 2.21 | 0.68 |
| 4:EF:122:LEU:HB3 | 4:EF:139:VAL:HB | 1.75 | 0.68 |
| 4:EF:168:PHE:HA | 4:EG:163:SER:HB3 | 1.73 | 0.68 |
| 2:GF:932:ARG:HG3 | 2:GF:1005:ARG:NH2 | 2.08 | 0.68 |
| 2:GF:214:ASP:HB2 | 2:GF:217:GLN:HE22 | 1.59 | 0.68 |
| 5:HB:501:LEU:HB3 | 5:HB:512:PRO:HB2 | 1.74 | 0.68 |
| 5:HC:194:LYS:O | 5:HC:242:VAL:HA | 1.93 | 0.68 |
| 5:HC:344:VAL:HG12 | 5:HC:349:TRP:H | 1.58 | 0.68 |
| 5:J:327:PRO:HG3 | 5:K:264:ARG:HD3 | 1.75 | 0.68 |
| 7:Q:476:ASP:HB2 | 5:FA:353:HIS:CD2 | 2.28 | 0.68 |
| 1:X:215:VAL:HG21 | 1:X:252:LEU:HD13 | 1.75 | 0.68 |
| 13:YA:36[D]:PRO:HG3 | 13:YA:45[D]:MET:HB2 | 1.74 | 0.68 |
| 13:YB:112[C]:GLU:HA | 13:YB:113[C]:GLY:N | 2.07 | 0.68 |
| 13:YB:321[A]:LYS:HD3 | 13:YC:452[A]:GLY:HA2 | 1.74 | 0.68 |
| 13:YB:558[A]:SER:HB3 | 13:YC:551[A]:THR:HG22 | 1.75 | 0.68 |
| 14:YD:17[D]:PHE:CD2 | 14:YD:23[D]:TRP:HA | 2.28 | 0.68 |
| 14:YE:17[F]:PHE:CD2 | 14:YE:23[F]:TRP:HA | 2.28 | 0.68 |
| 14:YE:184[F]:LYS:NZ | 14:YE:201[F]:ASP:OD2 | 2.26 | 0.68 |
| 14:YE:17[A]:PHE:CD2 | 14:YE:23[A]:TRP:HA | 2.27 | 0.68 |
| 14:YF:184[E]:LYS:NZ | 14:YF:201[E]:ASP:OD2 | 2.26 | 0.68 |
| 1:A:66:TYR:CE1 | 1:B:21:PHE:HB2 | 2.27 | 0.68 |
| 5:AD:327:PRO:HG3 | 5:AE:264:ARG:HD3 | 1.75 | 0.68 |
| 1:B:612:THR:HG22 | 1:B:614:GLU:H | 1.58 | 0.68 |
| 7:AJ:303:GLU:HA | 7:BA:309:ALA:HB3 | 1.74 | 0.68 |
| 1:BH:506:LYS:O | 1:BH:509:SER:OG | 2.11 | 0.68 |
| 1:BI:49:GLU:HA | 1:BI:54:ASN:HD22 | 1.57 | 0.68 |
| 2:BJ:1025:PRO:O | 2:BJ:1026:THR:HG22 | 1.92 | 0.68 |
| 2:BJ:241:SER:OG | 2:BJ:315:ASP:OD1 | 2.10 | 0.68 |
| 5:CF:397:ASP:O | 5:CF:401:ASP:N | 2.19 | 0.68 |
| 2:EC:251:ASP:OD2 | 2:EC:252:LYS:NZ | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:433:ASN:OD1 | 2:EC:434:MET:N | 2.25 | 0.68 |
| 2:EC:174:HIS:HD1 | 2:EC:508:TYR:HH | 1.40 | 0.68 |
| 10:GA:351:ILE:HG23 | 10:GA:352:ILE:HG23 | 1.75 | 0.68 |
| 5:HC:150:GLN:O | 5:HC:151:ILE:HG13 | 1.94 | 0.68 |
| 7:HI:50:ALA:HA | 7:HI:56:GLY:HA3 | 1.74 | 0.68 |
| 5:I:501:LEU:HB3 | 5:I:512:PRO:HB2 | 1.74 | 0.68 |
| 5:J:194:LYS:O | 5:J:242:VAL:HA | 1.93 | 0.68 |
| 1:Y:139:SER:OG | 1:Y:141:ASN:OD1 | 2.04 | 0.68 |
| 13:YA:81[C]:ARG:NH2 | 13:YA:101[C]:GLY:HA2 | 2.09 | 0.68 |
| 13:YA:112[B]:GLU:HA | 13:YA:113[B]:GLY:N | 2.07 | 0.68 |
| 14:YD:184[B]:LYS:NZ | 14:YD:201[B]:ASP:OD2 | 2.26 | 0.68 |
| 14:YD:211[B]:MET:HE1 | 14:YD:231[B]:ALA:HB2 | 1.75 | 0.68 |
| 14:YF:211[A]:MET:HE1 | 14:YF:231[A]:ALA:HB2 | 1.74 | 0.68 |
| 2:Z:214:ASP:HB2 | 2:Z:217:GLN:HE22 | 1.58 | 0.68 |
| 5:AD:344:VAL:HG12 | 5:AD:349:TRP:H | 1.58 | 0.68 |
| 12:BG:212:THR:OG1 | 12:BG:251:GLY:O | 2.12 | 0.68 |
| 2:BJ:214:ASP:HB2 | 2:BJ:217:GLN:HE22 | 1.59 | 0.68 |
| 2:BJ:444:SER:OG | 2:BJ:487:MET:SD | 2.49 | 0.68 |
| 5:CG:194:LYS:O | 5:CG:242:VAL:HA | 1.93 | 0.68 |
| 5:CH:323:THR:HG23 | 5:CH:359:GLU:HB2 | 1.74 | 0.68 |
| 12:DJ:24:CYS:HB3 | 12:DJ:125:ILE:HG21 | 1.75 | 0.68 |
| 5:EI:331:CYS:HA | 5:EI:349:TRP:HZ2 | 1.56 | 0.68 |
| 5:EJ:323:THR:HG23 | 5:EJ:359:GLU:HB2 | 1.76 | 0.68 |
| 5:EJ:305:ASN:ND2 | 5:FA:255:ARG:O | 2.26 | 0.68 |
| 5:EJ:391:GLY:HA3 | 5:FA:390:LEU:HD13 | 1.73 | 0.68 |
| 1:GE:612:THR:HG22 | 1:GE:614:GLU:H | 1.58 | 0.68 |
| 2:EC:529:SER:OG | 3:GH:233:GLN:OE1 | 2.12 | 0.68 |
| 4:GI:168:PHE:HA | 4:GJ:163:SER:HB3 | 1.74 | 0.68 |
| 5:HD:194:LYS:HB2 | 5:HD:243:GLN:HB2 | 1.75 | 0.68 |
| 7:HJ:166:GLN:HA | 7:HJ:170:ILE:HD12 | 1.74 | 0.68 |
| 8:R:95:GLN:NE2 | 8:IA:162:TRP:O | 2.25 | 0.68 |
| 5:J:311:VAL:HG11 | 5:J:321:ALA:H | 1.58 | 0.68 |
| 5:J:594:THR:HB | 5:K:490:TRP:HB2 | 1.75 | 0.68 |
| 13:YC:112[F]:GLU:HA | 13:YC:113[F]:GLY:N | 2.07 | 0.68 |
| 14:YD:17[C]:PHE:CD2 | 14:YD:23[C]:TRP:HA | 2.27 | 0.68 |
| 14:YD:17[E]:PHE:CD2 | 14:YD:23[E]:TRP:HA | 2.27 | 0.68 |
| 14:YE:211[A]:MET:HE1 | 14:YE:231[A]:ALA:HB2 | 1.75 | 0.68 |
| 2:Z:217:GLN:N | 2:Z:217:GLN:OE1 | 2.27 | 0.68 |
| 2:Z:824:GLN:O | 2:Z:825:GLU:HG2 | 1.94 | 0.68 |
| 5:AD:391:GLY:HA3 | 5:AE:390:LEU:HD13 | 1.74 | 0.68 |
| 1:BH:127:ARG:N | 1:BH:150:ASP:OD1 | 2.25 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:312:THR:HB | 2:BJ:319:TYR:HB2 | 1.75 | 0.68 |
| 2:C:217:GLN:N | 2:C:217:GLN:OE1 | 2.27 | 0.68 |
| 10:DH:351:ILE:HG23 | 10:DH:352:ILE:HG23 | 1.75 | 0.68 |
| 1:EB:49:GLU:HA | 1:EB:54:ASN:HD22 | 1.57 | 0.68 |
| 2:EC:217:GLN:OE1 | 2:EC:217:GLN:N | 2.27 | 0.68 |
| 2:EC:332:SER:OG | 2:EC:333:ASN:O | 2.11 | 0.68 |
| 2:EC:824:GLN:O | 2:EC:825:GLU:HG2 | 1.94 | 0.68 |
| 5:EI:406:LEU:O | 5:FA:409:SER:HA | 1.93 | 0.68 |
| 7:FF:117:THR:HG23 | 7:FF:120:LYS:H | 1.57 | 0.68 |
| 7:FF:193:LEU:HD13 | 7:FG:206:GLU:HG3 | 1.76 | 0.68 |
| 1:GD:66:TYR:CE1 | 1:GE:21:PHE:HB2 | 2.27 | 0.68 |
| 5:HD:339:GLU:HB2 | 6:HE:171:TYR:HB2 | 1.76 | 0.68 |
| 7:HH:448:ALA:N | 7:HI:485:ASN:OD1 | 2.27 | 0.68 |
| 1:GE:76:TYR:OH | 11:IE:29:PHE:O | 2.11 | 0.68 |
| 10:U:351:ILE:HG23 | 10:U:352:ILE:HG23 | 1.75 | 0.68 |
| 1:Y:38:ASN:OD1 | 1:Y:39:GLY:N | 2.27 | 0.68 |
| 13:YA:112[C]:GLU:HA | 13:YA:113[C]:GLY:N | 2.07 | 0.68 |
| 13:YA:112[E]:GLU:HA | 13:YA:113[E]:GLY:N | 2.07 | 0.68 |
| 13:YA:405[E]:ASP:OD1 | 13:YC:397[E]:SER:OG | 2.10 | 0.68 |
| 13:YB:112[A]:GLU:HA | 13:YB:113[A]:GLY:N | 2.07 | 0.68 |
| 13:YB:321[B]:LYS:HD3 | 13:YC:452[B]:GLY:HA2 | 1.74 | 0.68 |
| 13:YC:36[A]:PRO:HG3 | 13:YC:45[A]:MET:HB2 | 1.73 | 0.68 |
| 13:YC:36[C]:PRO:HG3 | 13:YC:45[C]:MET:HB2 | 1.75 | 0.68 |
| 14:YD:184[F]:LYS:NZ | 14:YD:201[F]:ASP:OD2 | 2.26 | 0.68 |
| 14:YE:184[D]:LYS:NZ | 14:YE:201[D]:ASP:OD2 | 2.26 | 0.68 |
| 14:YF:211[D]:MET:HE1 | 14:YF:231[D]:ALA:HB2 | 1.75 | 0.68 |
| 14:YF:36[D]:THR:HG22 | 14:YF:37[D]:THR:HG23 | 1.75 | 0.68 |
| 2:Z:58:ASN:OD1 | 2:Z:60:GLY:N | 2.23 | 0.68 |
| 1:B:174:ARG:HH21 | 1:B:269:VAL:HG21 | 1.58 | 0.68 |
| 7:BA:496:ARG:NH1 | 7:BA:501:THR:OG1 | 2.27 | 0.68 |
| 10:BE:351:ILE:HG23 | 10:BE:352:ILE:HG23 | 1.75 | 0.68 |
| 1:BH:215:VAL:HG21 | 1:BH:252:LEU:HD13 | 1.75 | 0.68 |
| 2:BJ:1000:THR:HA | 5:CF:18:TYR:HA | 1.76 | 0.68 |
| 2:BJ:433:ASN:ND2 | 2:BJ:513:PHE:HA | 2.09 | 0.68 |
| 2:C:433:ASN:OD1 | 2:C:434:MET:N | 2.25 | 0.68 |
| 5:CG:391:GLY:HA3 | 5:CH:390:LEU:HD13 | 1.74 | 0.68 |
| 1:EB:358:GLN:HB2 | 1:EB:379:LYS:HB3 | 1.76 | 0.68 |
| 2:EC:433:ASN:ND2 | 2:EC:513:PHE:HA | 2.09 | 0.68 |
| 5:EJ:265:LEU:HB3 | 5:EJ:281:TYR:HB3 | 1.75 | 0.68 |
| 4:H:122:LEU:HB3 | 4:H:139:VAL:HB | 1.75 | 0.68 |
| 5:J:331:CYS:HA | 5:J:349:TRP:HZ2 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:50:ALA:HA | 7:P:56:GLY:HA3 | 1.74 | 0.68 |
| 13:YA:81[E]:ARG:NH2 | 13:YA:101[E]:GLY:HA2 | 2.07 | 0.68 |
| 13:YB:81[E]:ARG:NH2 | 13:YB:101[E]:GLY:HA2 | 2.07 | 0.68 |
| 13:YB:36[D]:PRO:HG3 | 13:YB:45[D]:MET:HB2 | 1.74 | 0.68 |
| 13:YB:468[B]:ASP:OD2 | 13:YC:461[B]:SER:OG | 2.11 | 0.68 |
| 13:YC:112[D]:GLU:HA | 13:YC:113[D]:GLY:N | 2.07 | 0.68 |
| 13:YB:34[A]:LEU:HD13 | 14:YE:163[A]:THR:HG21 | 1.76 | 0.68 |
| 14:YF:17[B]:PHE:CD2 | 14:YF:23[B]:TRP:HA | 2.27 | 0.68 |
| 14:YF:17[D]:PHE:CD2 | 14:YF:23[D]:TRP:HA | 2.28 | 0.68 |
| 14:YF:36[B]:THR:HG22 | 14:YF:37[B]:THR:HG23 | 1.74 | 0.68 |
| 2:Z:932:ARG:HG3 | 2:Z:1005:ARG:NH2 | 2.08 | 0.68 |
| 1:A:127:ARG:N | 1:A:150:ASP:OD1 | 2.25 | 0.68 |
| 5:AC:144:GLU:HB3 | 5:AD:151:ILE:HD13 | 1.75 | 0.68 |
| 5:AE:72:THR:OG1 | 5:AE:101:THR:O | 2.11 | 0.68 |
| 5:AE:263:ILE:HG22 | 5:AE:381:ILE:HB | 1.76 | 0.68 |
| 7:AI:486:ASP:HB2 | 7:AJ:444:TYR:HB2 | 1.74 | 0.68 |
| 7:AJ:197:ALA:O | 7:AJ:201:GLN:HG3 | 1.93 | 0.68 |
| 1:B:38:ASN:OD1 | 1:B:39:GLY:N | 2.27 | 0.68 |
| 1:BH:63:ASN:ND2 | 1:BI:60:LEU:HB3 | 2.08 | 0.68 |
| 5:CF:312:ARG:O | 5:CF:382:ASN:N | 2.24 | 0.68 |
| 5:CG:31:ASP:O | 5:CG:35:TYR:N | 2.26 | 0.68 |
| 1:EB:612:THR:HG22 | 1:EB:614:GLU:H | 1.58 | 0.68 |
| 2:EC:174:HIS:ND1 | 2:EC:508:TYR:OH | 2.26 | 0.68 |
| 2:EC:58:ASN:OD1 | 2:EC:60:GLY:N | 2.23 | 0.68 |
| 2:EC:770:ILE:HG22 | 2:EC:842:VAL:H | 1.58 | 0.68 |
| 4:EF:64:THR:HA | 4:EG:84:ARG:HE | 1.58 | 0.68 |
| 4:EG:168:PHE:HA | 4:EH:163:SER:HB3 | 1.75 | 0.68 |
| 5:EJ:311:VAL:HG11 | 5:EJ:321:ALA:H | 1.58 | 0.68 |
| 5:FA:72:THR:OG1 | 5:FA:101:THR:O | 2.11 | 0.68 |
| 1:GE:174:ARG:HH21 | 1:GE:269:VAL:HG21 | 1.58 | 0.68 |
| 1:GE:358:GLN:HB2 | 1:GE:379:LYS:HB3 | 1.76 | 0.68 |
| 2:GF:312:THR:HB | 2:GF:319:TYR:HB2 | 1.75 | 0.68 |
| 10:GA:143:PHE:CD2 | 10:ID:349:ARG:HD3 | 2.27 | 0.68 |
| 5:K:323:THR:HG23 | 5:K:359:GLU:HB2 | 1.74 | 0.68 |
| 7:Q:496:ARG:NH1 | 7:Q:501:THR:OG1 | 2.26 | 0.68 |
| 13:YA:81[B]:ARG:NH2 | 13:YA:101[B]:GLY:HA2 | 2.09 | 0.68 |
| 13:YA:430[C]:ARG:NH1 | 13:YC:434[C]:THR:OG1 | 2.26 | 0.68 |
| 13:YC:112[A]:GLU:HA | 13:YC:113[A]:GLY:N | 2.07 | 0.68 |
| 13:YC:112[E]:GLU:HA | 13:YC:113[E]:GLY:N | 2.07 | 0.68 |
| 14:YF:184[B]:LYS:NZ | 14:YF:201[B]:ASP:OD2 | 2.26 | 0.68 |
| 14:YF:17[E]:PHE:CD2 | 14:YF:23[E]:TRP:HA | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:193:LEU:HD13 | 7:BA:206:GLU:HG3 | 1.76 | 0.68 |
| 10:BE:236:GLU:O | 10:BE:287:VAL:N | 2.27 | 0.68 |
| 4:CC:122:LEU:HB3 | 4:CC:139:VAL:HB | 1.75 | 0.68 |
| 5:CG:594:THR:HB | 5:CH:490:TRP:HB2 | 1.75 | 0.68 |
| 7:DB:193:LEU:HD11 | 7:DC:207:GLY:HA2 | 1.74 | 0.68 |
| 7:DC:50:ALA:HA | 7:DC:56:GLY:HA3 | 1.74 | 0.68 |
| 7:DC:36:ILE:HG21 | 7:DD:18:PHE:HZ | 1.58 | 0.68 |
| 10:DH:236:GLU:O | 10:DH:287:VAL:N | 2.27 | 0.68 |
| 2:EC:241:SER:OG | 2:EC:315:ASP:OD1 | 2.10 | 0.68 |
| 2:EC:752:TYR:OH | 2:EC:878:ASP:OD2 | 2.11 | 0.68 |
| 7:FF:50:ALA:HA | 7:FF:56:GLY:HA3 | 1.74 | 0.68 |
| 7:FF:512:THR:HA | 7:FG:442:MET:HA | 1.76 | 0.68 |
| 4:G:122:LEU:HB3 | 4:G:139:VAL:HB | 1.75 | 0.68 |
| 1:GD:63:ASN:ND2 | 1:GE:60:LEU:HB3 | 2.09 | 0.68 |
| 2:GF:174:HIS:ND1 | 2:GF:508:TYR:OH | 2.26 | 0.68 |
| 2:GF:824:GLN:O | 2:GF:825:GLU:HG2 | 1.94 | 0.68 |
| 3:GG:47:TRP:CH2 | 3:GG:58:PRO:HB3 | 2.29 | 0.68 |
| 5:HB:339:GLU:HG2 | 6:HF:173:THR:HB | 1.75 | 0.68 |
| 7:HJ:64:GLN:O | 7:HJ:68:ASP:N | 2.27 | 0.68 |
| 13:YA:430[B]:ARG:NH1 | 13:YC:434[B]:THR:OG1 | 2.27 | 0.68 |
| 13:YA:36[F]:PRO:HG3 | 13:YA:45[F]:MET:HB2 | 1.74 | 0.68 |
| 13:YB:81[F]:ARG:NH2 | 13:YB:101[F]:GLY:HA2 | 2.09 | 0.68 |
| 14:YD:17[F]:PHE:CD2 | 14:YD:23[F]:TRP:HA | 2.28 | 0.68 |
| 14:YD:36[A]:THR:HG22 | 14:YD:37[A]:THR:HG23 | 1.74 | 0.68 |
| 14:YD:36[D]:THR:HG22 | 14:YD:37[D]:THR:HG23 | 1.75 | 0.68 |
| 14:YD:288[F]:TYR:OH | 14:YD:371[F]:LYS:NZ | 2.27 | 0.68 |
| 13:YB:34[B]:LEU:HD13 | 14:YE:163[B]:THR:HG21 | 1.75 | 0.68 |
| 4:AA:122:LEU:HB3 | 4:AA:139:VAL:HB | 1.75 | 0.68 |
| 5:AD:594:THR:HB | 5:AE:490:TRP:HB2 | 1.75 | 0.68 |
| 5:K:353:HIS:CD2 | 7:BA:476:ASP:HB2 | 2.28 | 0.68 |
| 2:BJ:217:GLN:OE1 | 2:BJ:217:GLN:N | 2.27 | 0.68 |
| 5:CG:150:GLN:O | 5:CG:151:ILE:HG13 | 1.94 | 0.68 |
| 5:CF:316:ILE:HG23 | 5:CG:315:GLY:HA3 | 1.74 | 0.68 |
| 5:CG:327:PRO:HG3 | 5:CH:264:ARG:HD3 | 1.76 | 0.68 |
| 5:CG:323:THR:HG23 | 5:CG:359:GLU:HB2 | 1.76 | 0.68 |
| 5:CG:594:THR:OG1 | 5:CH:517:GLY:N | 2.27 | 0.68 |
| 7:DD:64:GLN:O | 7:DD:68:ASP:N | 2.27 | 0.68 |
| 5:CG:196:ARG:NH2 | 7:DD:9:VAL:HG12 | 2.08 | 0.68 |
| 4:F:113:ASN:HD22 | 4:G:103:LEU:HD21 | 1.59 | 0.68 |
| 3:E:155:LYS:HE2 | 2:GF:474:GLU:HB3 | 1.75 | 0.68 |
| 5:HB:459:ILE:HD11 | 5:HD:463:ALA:HB2 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:323:THR:HG23 | 5:HC:359:GLU:HB2 | 1.76 | 0.68 |
| 10:ID:351:ILE:HG23 | 10:ID:352:ILE:HG23 | 1.75 | 0.68 |
| 11:IE:178:ASN:N | 14:YD:217[F]:SER:O | 2.25 | 0.68 |
| 5:J:150:GLN:O | 5:J:151:ILE:HG13 | 1.94 | 0.68 |
| 5:J:305:ASN:ND2 | 5:K:255:ARG:O | 2.26 | 0.68 |
| 13:YA:430[F]:ARG:NH1 | 13:YC:434[F]:THR:OG1 | 2.26 | 0.68 |
| 14:YE:36[C]:THR:HG22 | 14:YE:37[C]:THR:HG23 | 1.74 | 0.68 |
| 5:AD:265:LEU:HB3 | 5:AD:281:TYR:HB3 | 1.75 | 0.68 |
| 1:BI:38:ASN:OD1 | 1:BI:39:GLY:N | 2.27 | 0.68 |
| 2:BJ:141:THR:HG22 | 2:BJ:547:ASN:H | 1.57 | 0.68 |
| 2:BJ:770:ILE:HG22 | 2:BJ:842:VAL:H | 1.59 | 0.68 |
| 2:C:824:GLN:N | 2:C:837:GLU:OE2 | 2.24 | 0.68 |
| 5:CG:320:LEU:HD23 | 5:CG:358:VAL:HG23 | 1.76 | 0.68 |
| 5:CG:331:CYS:HA | 5:CG:349:TRP:HZ2 | 1.59 | 0.68 |
| 5:CH:194:LYS:HB2 | 5:CH:243:GLN:HB2 | 1.75 | 0.68 |
| 5:CG:305:ASN:ND2 | 5:CH:255:ARG:O | 2.26 | 0.68 |
| 5:CG:326:MET:HE3 | 5:CH:279:SER:HA | 1.76 | 0.68 |
| 3:D:47:TRP:CH2 | 3:D:58:PRO:HB3 | 2.29 | 0.68 |
| 1:EB:619:GLN:HG2 | 1:EB:620:THR:HG23 | 1.75 | 0.68 |
| 5:EI:200:LEU:HD23 | 5:EI:210:SER:HA | 1.76 | 0.68 |
| 5:EJ:331:CYS:HA | 5:EJ:349:TRP:HZ2 | 1.59 | 0.68 |
| 5:EJ:344:VAL:HG12 | 5:EJ:349:TRP:H | 1.58 | 0.68 |
| 7:HH:486:ASP:HB2 | 7:HI:444:TYR:HB2 | 1.74 | 0.68 |
| 5:J:153:LYS:O | 5:J:154:ILE:HG13 | 1.94 | 0.68 |
| 5:J:323:THR:HG23 | 5:J:359:GLU:HB2 | 1.76 | 0.68 |
| 7:O:188:GLN:HG3 | 7:Q:192:GLN:HB2 | 1.75 | 0.68 |
| 13:YA:112[D]:GLU:HA | 13:YA:113[D]:GLY:N | 2.07 | 0.68 |
| 13:YA:405[D]:ASP:OD1 | 13:YC:397[D]:SER:OG | 2.11 | 0.68 |
| 13:YA:430[A]:ARG:NH1 | 13:YC:434[A]:THR:OG1 | 2.27 | 0.68 |
| 13:YB:112[B]:GLU:HA | 13:YB:113[B]:GLY:N | 2.07 | 0.68 |
| 13:YB:61[B]:ILE:HG22 | 13:YC:76[B]:PRO:HA | 1.76 | 0.68 |
| 13:YB:81[A]:ARG:NH2 | 13:YB:101[A]:GLY:HA2 | 2.09 | 0.68 |
| 13:YC:57[C]:VAL:HG11 | 13:YC:76[C]:PRO:HD3 | 1.76 | 0.68 |
| 14:YD:211[C]:MET:HE1 | 14:YD:231[C]:ALA:HB2 | 1.76 | 0.68 |
| 14:YF:245[B]:ARG:NE | 14:YF:246[B]:ASP:OD1 | 2.25 | 0.68 |
| 5:AD:331:CYS:HA | 5:AD:349:TRP:HZ2 | 1.59 | 0.67 |
| 1:BH:90:VAL:O | 1:BH:94:GLN:N | 2.26 | 0.67 |
| 2:BJ:509:TYR:HB3 | 3:EE:229:LEU:HD23 | 1.76 | 0.67 |
| 2:C:251:ASP:OD2 | 2:C:252:LYS:NZ | 2.26 | 0.67 |
| 5:CH:263:ILE:HG22 | 5:CH:381:ILE:HB | 1.76 | 0.67 |
| 5:CH:338:ASP:HB3 | 5:CH:349:TRP:CD1 | 2.30 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:20:PRO:HG3 | 7:DB:29:ILE:HG13 | 1.76 | 0.67 |
| 7:DB:170:ILE:HD13 | 7:DC:172:LEU:HD22 | 1.75 | 0.67 |
| 8:BB:43:ALA:HB1 | 8:DE:138:GLY:HA3 | 1.75 | 0.67 |
| 2:EC:233:LEU:HD12 | 2:EC:391:ARG:HB2 | 1.75 | 0.67 |
| 5:EI:397:ASP:O | 5:EI:401:ASP:N | 2.19 | 0.67 |
| 5:EJ:320:LEU:HD23 | 5:EJ:358:VAL:HG23 | 1.77 | 0.67 |
| 7:FF:41:PRO:O | 7:FF:45:ASN:ND2 | 2.27 | 0.67 |
| 7:FG:496:ARG:NH1 | 7:FG:501:THR:OG1 | 2.27 | 0.67 |
| 12:GC:147:ASN:OD1 | 12:GC:148:ILE:N | 2.28 | 0.67 |
| 2:GF:433:ASN:ND2 | 2:GF:513:PHE:HA | 2.09 | 0.67 |
| 5:HC:331:CYS:HA | 5:HC:349:TRP:HZ2 | 1.59 | 0.67 |
| 12:IF:147:ASN:OD1 | 12:IF:148:ILE:N | 2.28 | 0.67 |
| 5:I:144:GLU:HB3 | 5:J:151:ILE:HD13 | 1.75 | 0.67 |
| 7:O:207:GLY:HA2 | 7:Q:193:LEU:HD11 | 1.76 | 0.67 |
| 7:P:41:PRO:O | 7:P:45:ASN:ND2 | 2.27 | 0.67 |
| 7:O:57:ILE:HG22 | 7:P:55:LYS:HB3 | 1.76 | 0.67 |
| 8:S:95:GLN:NE2 | 8:IB:162:TRP:O | 2.26 | 0.67 |
| 8:S:96:GLY:O | 8:FI:56:ARG:NH2 | 2.27 | 0.67 |
| 13:YA:408[C]:GLY:N | 13:YA:410[C]:GLU:OE2 | 2.27 | 0.67 |
| 13:YB:321[E]:LYS:HD3 | 13:YC:452[E]:GLY:HA2 | 1.74 | 0.67 |
| 13:YA:430[D]:ARG:NH1 | 13:YC:434[D]:THR:OG1 | 2.27 | 0.67 |
| 13:YC:36[F]:PRO:HG3 | 13:YC:45[F]:MET:HB2 | 1.74 | 0.67 |
| 13:YC:81[C]:ARG:NH2 | 13:YC:101[C]:GLY:HA2 | 2.09 | 0.67 |
| 13:YC:81[D]:ARG:NH2 | 13:YC:101[D]:GLY:HA2 | 2.09 | 0.67 |
| 14:YD:36[E]:THR:HG22 | 14:YD:37[E]:THR:HG23 | 1.75 | 0.67 |
| 14:YD:36[F]:THR:HG22 | 14:YD:37[F]:THR:HG23 | 1.74 | 0.67 |
| 13:YB:34[D]:LEU:HD13 | 14:YE:163[D]:THR:HG21 | 1.75 | 0.67 |
| 14:YE:17[D]:PHE:CD2 | 14:YE:23[D]:TRP:HA | 2.28 | 0.67 |
| 2:Z:233:LEU:HD12 | 2:Z:391:ARG:HB2 | 1.75 | 0.67 |
| 4:AA:64:THR:HA | 4:AB:84:ARG:HE | 1.58 | 0.67 |
| 5:AE:338:ASP:HB3 | 5:AE:349:TRP:CD1 | 2.29 | 0.67 |
| 7:AI:102:THR:HG22 | 7:AI:105:GLU:HG3 | 1.76 | 0.67 |
| 1:B:358:GLN:HB2 | 1:B:379:LYS:HB3 | 1.76 | 0.67 |
| 7:BA:64:GLN:O | 7:BA:68:ASP:N | 2.27 | 0.67 |
| 2:BJ:233:LEU:HD12 | 2:BJ:391:ARG:HB2 | 1.75 | 0.67 |
| 2:C:312:THR:HB | 2:C:319:TYR:HB2 | 1.75 | 0.67 |
| 4:CE:122:LEU:HB3 | 4:CE:139:VAL:HB | 1.75 | 0.67 |
| 5:CH:175:THR:O | 5:CH:232:LEU:N | 2.26 | 0.67 |
| 5:CH:62:ALA:HB1 | 5:CH:82:PRO:HG3 | 1.76 | 0.67 |
| 1:EB:38:ASN:OD1 | 1:EB:39:GLY:N | 2.27 | 0.67 |
| 4:EH:122:LEU:HB3 | 4:EH:139:VAL:HB | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:507:ASP:OD1 | 5:EJ:511:ASN:N | 2.22 | 0.67 |
| 6:FC:70:ILE:HG12 | 6:FD:73:ASN:HA | 1.77 | 0.67 |
| 8:FI:162:TRP:O | 8:IB:95:GLN:NE2 | 2.26 | 0.67 |
| 12:GC:212:THR:OG1 | 12:GC:251:GLY:O | 2.12 | 0.67 |
| 2:GF:1000:THR:HA | 5:HB:18:TYR:HA | 1.75 | 0.67 |
| 7:HH:207:GLY:HA2 | 7:HJ:193:LEU:HD11 | 1.76 | 0.67 |
| 5:I:407:TYR:CE1 | 5:K:407:TYR:HB2 | 2.29 | 0.67 |
| 5:J:326:MET:HE3 | 5:K:279:SER:HA | 1.76 | 0.67 |
| 7:Q:64:GLN:O | 7:Q:68:ASP:N | 2.27 | 0.67 |
| 13:YB:57[C]:VAL:HG11 | 13:YB:76[C]:PRO:HD3 | 1.76 | 0.67 |
| 14:YD:245[D]:ARG:NE | 14:YD:246[D]:ASP:OD1 | 2.25 | 0.67 |
| 14:YE:260[A]:ASP:OD1 | 14:YE:262[A]:SER:N | 2.27 | 0.67 |
| 14:YE:288[D]:TYR:OH | 14:YE:371[D]:LYS:NZ | 2.27 | 0.67 |
| 5:AD:150:GLN:O | 5:AD:151:ILE:HG13 | 1.94 | 0.67 |
| 5:AE:353:HIS:CD2 | 7:FG:476:ASP:HB2 | 2.30 | 0.67 |
| 2:C:174:HIS:HD1 | 2:C:508:TYR:HH | 1.40 | 0.67 |
| 2:C:433:ASN:ND2 | 2:C:513:PHE:HA | 2.09 | 0.67 |
| 2:C:824:GLN:O | 2:C:825:GLU:HG2 | 1.94 | 0.67 |
| 4:CD:275:ALA:O | 4:CE:282:GLN:NE2 | 2.27 | 0.67 |
| 7:DB:199:VAL:HA | 7:DD:212:PRO:HB3 | 1.75 | 0.67 |
| 5:EJ:72:THR:OG1 | 5:EJ:101:THR:O | 2.13 | 0.67 |
| 5:FA:130:PHE:HB3 | 5:FA:151:ILE:HG22 | 1.76 | 0.67 |
| 1:GE:553:VAL:N | 1:GE:593:GLY:O | 2.23 | 0.67 |
| 5:HC:72:THR:OG1 | 5:HC:101:THR:O | 2.13 | 0.67 |
| 5:HC:198:ASN:HD22 | 5:HD:194:LYS:HD3 | 1.57 | 0.67 |
| 5:HC:326:MET:HE3 | 5:HD:279:SER:HA | 1.76 | 0.67 |
| 5:I:200:LEU:HD23 | 5:I:210:SER:HA | 1.76 | 0.67 |
| 12:GC:211:HIS:HE1 | 12:IF:168:ALA:N | 1.92 | 0.67 |
| 13:YB:468[E]:ASP:OD2 | 13:YC:461[E]:SER:OG | 2.11 | 0.67 |
| 13:YB:558[F]:SER:HB3 | 13:YC:551[F]:THR:HG22 | 1.75 | 0.67 |
| 14:YD:245[F]:ARG:NE | 14:YD:246[F]:ASP:OD1 | 2.26 | 0.67 |
| 13:YB:34[E]:LEU:HD13 | 14:YE:163[E]:THR:HG21 | 1.75 | 0.67 |
| 14:YF:211[F]:MET:HE1 | 14:YF:231[F]:ALA:HB2 | 1.74 | 0.67 |
| 14:YF:260[E]:ASP:OD1 | 14:YF:262[E]:SER:N | 2.27 | 0.67 |
| 4:AB:122:LEU:HB3 | 4:AB:139:VAL:HB | 1.75 | 0.67 |
| 5:AD:323:THR:HG23 | 5:AD:359:GLU:HB2 | 1.76 | 0.67 |
| 5:AD:320:LEU:HD23 | 5:AD:358:VAL:HG23 | 1.76 | 0.67 |
| 1:B:243:ILE:HD11 | 1:B:252:LEU:HB3 | 1.75 | 0.67 |
| 1:BH:517:PHE:N | 1:BH:536:TYR:O | 2.24 | 0.67 |
| 1:BI:174:ARG:HH21 | 1:BI:269:VAL:HG21 | 1.58 | 0.67 |
| 2:C:174:HIS:ND1 | 2:C:508:TYR:OH | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:340:PRO:HA | 2:C:345:TYR:CE1 | 2.30 | 0.67 |
| 4:CC:103:LEU:HD21 | 4:CE:113:ASN:HD22 | 1.58 | 0.67 |
| 5:CG:251:VAL:O | 5:CH:161:ASN:ND2 | 2.27 | 0.67 |
| 5:CH:72:THR:OG1 | 5:CH:101:THR:O | 2.11 | 0.67 |
| 2:EC:236:THR:HG23 | 2:EC:367:LYS:HE3 | 1.76 | 0.67 |
| 2:EC:344:THR:OG1 | 2:EC:347:GLU:OE1 | 2.09 | 0.67 |
| 4:EF:84:ARG:HE | 4:EH:64:THR:HA | 1.58 | 0.67 |
| 5:EJ:360:THR:HA | 5:EJ:366:PRO:HB3 | 1.77 | 0.67 |
| 7:FE:20:PRO:HG3 | 7:FE:29:ILE:HG13 | 1.76 | 0.67 |
| 10:GA:236:GLU:O | 10:GA:287:VAL:N | 2.27 | 0.67 |
| 4:HA:122:LEU:HB3 | 4:HA:139:VAL:HB | 1.75 | 0.67 |
| 5:HC:320:LEU:HD23 | 5:HC:358:VAL:HG23 | 1.76 | 0.67 |
| 5:HD:175:THR:O | 5:HD:232:LEU:N | 2.26 | 0.67 |
| 7:HJ:496:ARG:NH1 | 7:HJ:501:THR:OG1 | 2.27 | 0.67 |
| 12:IF:24:CYS:HB3 | 12:IF:125:ILE:HG21 | 1.75 | 0.67 |
| 5:J:72:THR:OG1 | 5:J:101:THR:O | 2.13 | 0.67 |
| 1:Y:358:GLN:HB2 | 1:Y:379:LYS:HB3 | 1.76 | 0.67 |
| 13:YC:76[E]:PRO:HB3 | 13:YC:98[E]:GLY:CA | 2.25 | 0.67 |
| 14:YD:260[C]:ASP:OD1 | 14:YD:262[C]:SER:N | 2.28 | 0.67 |
| 14:YE:211[F]:MET:HE1 | 14:YE:231[F]:ALA:HB2 | 1.76 | 0.67 |
| 14:YF:260[A]:ASP:OD1 | 14:YF:262[A]:SER:N | 2.27 | 0.67 |
| 5:CG:153:LYS:O | 5:CG:154:ILE:HG13 | 1.94 | 0.67 |
| 5:CH:344:VAL:HG12 | 5:CH:349:TRP:HB3 | 1.77 | 0.67 |
| 6:CJ:52:ILE:HD11 | 6:DA:15:ALA:HB2 | 1.77 | 0.67 |
| 7:DB:69:GLY:HA2 | 7:DD:78:PRO:HB2 | 1.75 | 0.67 |
| 7:DD:371:ASP:OD1 | 7:DD:526:LYS:NZ | 2.23 | 0.67 |
| 12:DJ:212:THR:OG1 | 12:DJ:251:GLY:O | 2.12 | 0.67 |
| 2:EC:312:THR:HB | 2:EC:319:TYR:HB2 | 1.75 | 0.67 |
| 3:ED:47:TRP:CH2 | 3:ED:58:PRO:HB3 | 2.29 | 0.67 |
| 4:F:168:PHE:HA | 4:G:163:SER:HB3 | 1.76 | 0.67 |
| 5:FA:338:ASP:HB3 | 5:FA:349:TRP:CD1 | 2.29 | 0.67 |
| 5:FA:62:ALA:HB1 | 5:FA:82:PRO:HG3 | 1.76 | 0.67 |
| 7:FF:357:ASP:OD1 | 7:FG:339:ARG:NH2 | 2.26 | 0.67 |
| 9:FJ:59:ASP:HA | 9:FJ:62:PHE:HB3 | 1.77 | 0.67 |
| 12:GC:24:CYS:HB3 | 12:GC:125:ILE:HG21 | 1.75 | 0.67 |
| 1:GE:619:GLN:HG2 | 1:GE:620:THR:HG23 | 1.75 | 0.67 |
| 5:HB:24:ILE:HG13 | 5:HD:7:ILE:HD11 | 1.76 | 0.67 |
| 5:HD:72:THR:OG1 | 5:HD:101:THR:O | 2.11 | 0.67 |
| 5:J:360:THR:HA | 5:J:366:PRO:HB3 | 1.77 | 0.67 |
| 7:P:486:ASP:HB2 | 7:Q:444:TYR:HB2 | 1.76 | 0.67 |
| 1:Y:243:ILE:HD11 | 1:Y:252:LEU:HB3 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:260[E]:ASP:OD1 | 14:YD:262[E]:SER:N | 2.27 | 0.67 |
| 14:YE:245[D]:ARG:NE | 14:YE:246[D]:ASP:OD1 | 2.25 | 0.67 |
| 5:AD:318:GLN:HB3 | 6:AF:4:LEU:HG | 1.76 | 0.67 |
| 7:AJ:325:TYR:HD1 | 7:AJ:330:ARG:HA | 1.57 | 0.67 |
| 1:B:595:ILE:HG22 | 1:B:602:ILE:HA | 1.77 | 0.67 |
| 7:AI:188:GLN:HG3 | 7:BA:192:GLN:HB2 | 1.75 | 0.67 |
| 1:BI:595:ILE:HG22 | 1:BI:602:ILE:HA | 1.77 | 0.67 |
| 1:BI:619:GLN:HG2 | 1:BI:620:THR:HG23 | 1.75 | 0.67 |
| 2:BJ:824:GLN:O | 2:BJ:825:GLU:HG2 | 1.94 | 0.67 |
| 5:CG:360:THR:HA | 5:CG:366:PRO:HB3 | 1.77 | 0.67 |
| 5:CF:577:ASN:ND2 | 5:CG:529:ASN:OD1 | 2.23 | 0.67 |
| 5:CH:130:PHE:HB3 | 5:CH:151:ILE:HG22 | 1.76 | 0.67 |
| 7:DB:220:SER:OG | 7:DD:228:ILE:O | 2.08 | 0.67 |
| 11:DI:123:LEU:HD12 | 11:DI:135:ASP:HA | 1.77 | 0.67 |
| 1:EA:649:GLN:OE1 | 1:EA:649:GLN:N | 2.25 | 0.67 |
| 1:EA:417:LYS:HA | 1:EA:650:TYR:O | 1.95 | 0.67 |
| 5:EJ:153:LYS:O | 5:EJ:154:ILE:HG13 | 1.94 | 0.67 |
| 7:FE:211:SER:N | 7:FE:214:THR:OG1 | 2.28 | 0.67 |
| 7:FF:130:GLU:HG2 | 7:FG:139:ASN:HD21 | 1.59 | 0.67 |
| 2:GF:217:GLN:N | 2:GF:217:GLN:OE1 | 2.27 | 0.67 |
| 1:GE:230:ILE:HD13 | 2:GF:691:ARG:HG3 | 1.77 | 0.67 |
| 5:HC:265:LEU:HB3 | 5:HC:281:TYR:HB3 | 1.75 | 0.67 |
| 5:HD:338:ASP:HB3 | 5:HD:349:TRP:CD1 | 2.29 | 0.67 |
| 7:HI:41:PRO:O | 7:HI:45:ASN:ND2 | 2.27 | 0.67 |
| 12:IF:212:THR:OG1 | 12:IF:251:GLY:O | 2.12 | 0.67 |
| 5:K:194:LYS:HB2 | 5:K:243:GLN:HB2 | 1.75 | 0.67 |
| 6:M:17:PHE:O | 6:N:13:ARG:NH1 | 2.21 | 0.67 |
| 8:S:138:GLY:HA3 | 8:IB:43:ALA:HB1 | 1.76 | 0.67 |
| 13:YA:430[E]:ARG:NH1 | 13:YC:434[E]:THR:OG1 | 2.27 | 0.67 |
| 13:YB:408[A]:GLY:N | 13:YB:410[A]:GLU:OE2 | 2.28 | 0.67 |
| 13:YC:408[E]:GLY:N | 13:YC:410[E]:GLU:OE2 | 2.28 | 0.67 |
| 13:YA:550[E]:TRP:CD1 | 13:YC:554[E]:MET:HE2 | 2.29 | 0.67 |
| 14:YD:260[F]:ASP:OD1 | 14:YD:262[F]:SER:N | 2.27 | 0.67 |
| 14:YE:260[C]:ASP:OD1 | 14:YE:262[C]:SER:N | 2.28 | 0.67 |
| 14:YF:260[F]:ASP:OD1 | 14:YF:262[F]:SER:N | 2.27 | 0.67 |
| 14:YF:36[C]:THR:HG22 | 14:YF:37[C]:THR:HG23 | 1.75 | 0.67 |
| 2:Z:340:PRO:HA | 2:Z:345:TYR:CE1 | 2.30 | 0.67 |
| 5:AD:72:THR:OG1 | 5:AD:101:THR:O | 2.13 | 0.67 |
| 5:AE:270:LEU:HG | 6:AH:108:LEU:HD21 | 1.77 | 0.67 |
| 11:BF:123:LEU:HD12 | 11:BF:135:ASP:HA | 1.77 | 0.67 |
| 2:BJ:251:ASP:OD2 | 2:BJ:252:LYS:NZ | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:236:THR:HG23 | 2:BJ:367:LYS:HE3 | 1.77 | 0.67 |
| 2:BJ:58:ASN:OD1 | 2:BJ:60:GLY:N | 2.23 | 0.67 |
| 4:CC:113:ASN:HD22 | 4:CD:103:LEU:HD21 | 1.59 | 0.67 |
| 5:CG:72:THR:OG1 | 5:CG:101:THR:O | 2.13 | 0.67 |
| 7:DB:102:THR:HG22 | 7:DB:105:GLU:HG3 | 1.76 | 0.67 |
| 7:DB:193:LEU:HD13 | 7:DC:206:GLU:HG3 | 1.76 | 0.67 |
| 7:DD:496:ARG:NH1 | 7:DD:501:THR:OG1 | 2.27 | 0.67 |
| 1:EB:595:ILE:HG22 | 1:EB:602:ILE:HA | 1.77 | 0.67 |
| 2:EC:777:LEU:HD23 | 2:EC:809:TRP:CG | 2.30 | 0.67 |
| 4:EH:106:CYS:SG | 4:EH:149:ARG:NH2 | 2.67 | 0.67 |
| 5:FA:175:THR:O | 5:FA:232:LEU:N | 2.26 | 0.67 |
| 5:EI:407:TYR:CE1 | 5:FA:407:TYR:HB2 | 2.30 | 0.67 |
| 1:GE:595:ILE:HG22 | 1:GE:602:ILE:HA | 1.77 | 0.67 |
| 7:HI:193:LEU:HD13 | 7:HJ:206:GLU:HG3 | 1.76 | 0.67 |
| 10:ID:236:GLU:O | 10:ID:287:VAL:N | 2.27 | 0.67 |
| 10:U:236:GLU:O | 10:U:287:VAL:N | 2.27 | 0.67 |
| 13:YA:81[A]:ARG:NH2 | 13:YA:101[A]:GLY:HA2 | 2.09 | 0.67 |
| 13:YB:81[C]:ARG:NH2 | 13:YB:101[C]:GLY:HA2 | 2.09 | 0.67 |
| 13:YC:81[B]:ARG:NH2 | 13:YC:101[B]:GLY:HA2 | 2.09 | 0.67 |
| 13:YC:81[F]:ARG:NH2 | 13:YC:101[F]:GLY:HA2 | 2.09 | 0.67 |
| 14:YD:288[A]:TYR:OH | 14:YD:371[A]:LYS:NZ | 2.27 | 0.67 |
| 14:YE:260[F]:ASP:OD1 | 14:YE:262[F]:SER:N | 2.27 | 0.67 |
| 14:YE:36[E]:THR:HG22 | 14:YE:37[E]:THR:HG23 | 1.75 | 0.67 |
| 5:AE:62:ALA:HB1 | 5:AE:82:PRO:HG3 | 1.76 | 0.67 |
| 6:AF:12:SER:CB | 6:AH:6:ASN:HB3 | 2.25 | 0.67 |
| 2:C:389:ASN:HB3 | 2:C:392:THR:HG22 | 1.77 | 0.67 |
| 2:C:444:SER:OG | 2:C:487:MET:SD | 2.49 | 0.67 |
| 7:DB:18:PHE:HA | 7:DD:13:SER:HB2 | 1.76 | 0.67 |
| 7:DC:486:ASP:HB2 | 7:DD:444:TYR:HB2 | 1.76 | 0.67 |
| 7:DB:57:ILE:HG22 | 7:DC:55:LYS:HB3 | 1.77 | 0.67 |
| 8:BC:43:ALA:HB1 | 8:DF:138:GLY:HA3 | 1.76 | 0.67 |
| 9:DG:59:ASP:HA | 9:DG:62:PHE:HB3 | 1.77 | 0.67 |
| 1:EB:553:VAL:N | 1:EB:593:GLY:O | 2.23 | 0.67 |
| 2:EC:3:VAL:O | 2:EC:90:GLU:N | 2.26 | 0.67 |
| 1:EB:230:ILE:HD13 | 2:EC:691:ARG:HG3 | 1.77 | 0.67 |
| 5:EJ:150:GLN:O | 5:EJ:151:ILE:HG13 | 1.94 | 0.67 |
| 5:EJ:31:ASP:O | 5:EJ:35:TYR:N | 2.26 | 0.67 |
| 5:HB:406:LEU:O | 5:HD:409:SER:HA | 1.95 | 0.67 |
| 7:HH:20:PRO:HG3 | 7:HH:29:ILE:HG13 | 1.76 | 0.67 |
| 5:I:77:VAL:HG23 | 7:AJ:167:GLN:HE21 | 231.49 | 0.67 |
| 5:J:344:VAL:HG12 | 5:J:349:TRP:H | 1.58 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:62:ALA:HB1 | 5:K:82:PRO:HG3 | 1.76 | 0.67 |
| 7:O:141:VAL:HG22 | 7:P:139:ASN:HB2 | 1.76 | 0.67 |
| 11:V:129:ASN:HB2 | 11:V:132:VAL:HG12 | 1.77 | 0.67 |
| 12:W:212:THR:OG1 | 12:W:251:GLY:O | 2.12 | 0.67 |
| 1:X:553:VAL:N | 1:X:593:GLY:O | 2.21 | 0.67 |
| 1:X:417:LYS:HA | 1:X:650:TYR:O | 1.95 | 0.67 |
| 13:YA:403[D]:PHE:HB3 | 13:YC:399[D]:HIS:CD2 | 2.30 | 0.67 |
| 13:YA:57[C]:VAL:HG11 | 13:YA:76[C]:PRO:HD3 | 1.76 | 0.67 |
| 13:YB:61[D]:ILE:HA | 13:YC:76[D]:PRO:CA | 2.24 | 0.67 |
| 14:YD:260[B]:ASP:OD1 | 14:YD:262[B]:SER:N | 2.28 | 0.67 |
| 13:YB:34[F]:LEU:HD13 | 14:YE:163[F]:THR:HG21 | 1.76 | 0.67 |
| 14:YE:19[C]:SER:H | 14:YE:22[C]:ALA:HB3 | 1.60 | 0.67 |
| 14:YE:260[B]:ASP:OD1 | 14:YE:262[B]:SER:N | 2.27 | 0.67 |
| 14:YF:260[B]:ASP:OD1 | 14:YF:262[B]:SER:N | 2.27 | 0.67 |
| 2:Z:52:ASN:OD1 | 2:Z:53:GLN:N | 2.27 | 0.67 |
| 5:AD:507:ASP:OD1 | 5:AD:511:ASN:N | 2.22 | 0.67 |
| 7:AJ:486:ASP:HB2 | 7:BA:444:TYR:HB2 | 1.76 | 0.67 |
| 1:BH:337:GLN:HG3 | 1:BI:334:GLU:HG2 | 1.77 | 0.67 |
| 2:BJ:340:PRO:HA | 2:BJ:345:TYR:CE1 | 2.30 | 0.67 |
| 2:C:539:LEU:HB3 | 2:C:541:TYR:H | 1.60 | 0.67 |
| 7:DB:188:GLN:HG3 | 7:DD:192:GLN:HB2 | 1.76 | 0.67 |
| 1:EA:99:LEU:HG | 1:EA:211:ARG:HH12 | 1.59 | 0.67 |
| 1:EB:290:ASP:OD1 | 1:EB:291:THR:N | 2.28 | 0.67 |
| 1:EB:38:ASN:ND2 | 1:GD:264:GLN:OE1 | 2.27 | 0.67 |
| 2:EC:926:PRO:HG3 | 2:EC:969:TYR:CE2 | 2.30 | 0.67 |
| 5:EI:234:GLN:NE2 | 7:FG:9:VAL:HG21 | 2.10 | 0.67 |
| 2:GF:340:PRO:HA | 2:GF:345:TYR:CE1 | 2.30 | 0.67 |
| 2:GF:389:ASN:HB3 | 2:GF:392:THR:HG22 | 1.77 | 0.67 |
| 2:GF:67:PHE:HE2 | 2:GF:69:PHE:HB2 | 1.60 | 0.67 |
| 2:GF:777:LEU:HD23 | 2:GF:809:TRP:CG | 2.30 | 0.67 |
| 4:GI:113:ASN:HD22 | 4:GJ:103:LEU:HD21 | 1.60 | 0.67 |
| 5:HC:151:ILE:HD12 | 5:HC:152:ASP:N | 2.10 | 0.67 |
| 5:HD:344:VAL:HG12 | 5:HD:349:TRP:HB3 | 1.77 | 0.67 |
| 12:IF:177:TRP:HZ3 | 12:IF:220:SER:HB3 | 1.60 | 0.67 |
| 5:K:102:TRP:CE3 | 5:K:131:SER:HB2 | 2.30 | 0.67 |
| 8:R:64:ARG:HD3 | 8:IA:56:ARG:HD3 | 1.77 | 0.67 |
| 12:W:9:ASN:O | 12:W:13:ASN:ND2 | 2.28 | 0.67 |
| 12:W:147:ASN:OD1 | 12:W:148:ILE:N | 2.28 | 0.67 |
| 13:YA:81[D]:ARG:NH2 | 13:YA:101[D]:GLY:HA2 | 2.09 | 0.67 |
| 13:YA:76[E]:PRO:HB3 | 13:YA:98[E]:GLY:CA | 2.25 | 0.67 |
| 13:YB:34[C]:LEU:HD13 | 14:YE:163[C]:THR:HG21 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:36[C]:PRO:HG3 | 13:YB:45[C]:MET:HB2 | 1.75 | 0.67 |
| 13:YB:81[B]:ARG:NH2 | 13:YB:101[B]:GLY:HA2 | 2.09 | 0.67 |
| 14:YD:260[D]:ASP:OD1 | 14:YD:262[D]:SER:N | 2.28 | 0.67 |
| 14:YE:211[B]:MET:HE1 | 14:YE:231[B]:ALA:HB2 | 1.75 | 0.67 |
| 14:YE:260[D]:ASP:OD1 | 14:YE:262[D]:SER:N | 2.28 | 0.67 |
| 14:YE:288[E]:TYR:OH | 14:YE:371[E]:LYS:NZ | 2.27 | 0.67 |
| 14:YE:288[A]:TYR:OH | 14:YE:371[A]:LYS:NZ | 2.27 | 0.67 |
| 7:AI:448:ALA:N | 7:AJ:485:ASN:OD1 | 2.27 | 0.67 |
| 12:BG:147:ASN:OD1 | 12:BG:148:ILE:N | 2.28 | 0.67 |
| 1:BI:290:ASP:OD1 | 1:BI:291:THR:N | 2.28 | 0.67 |
| 2:BJ:67:PHE:HE2 | 2:BJ:69:PHE:HB2 | 1.60 | 0.67 |
| 3:CB:170:PRO:HB3 | 3:CB:188:TRP:CD1 | 2.30 | 0.67 |
| 7:DC:325:TYR:HD1 | 7:DC:330:ARG:HA | 1.57 | 0.67 |
| 1:EB:243:ILE:HD11 | 1:EB:252:LEU:HB3 | 1.75 | 0.67 |
| 2:EC:67:PHE:HE2 | 2:EC:69:PHE:HB2 | 1.60 | 0.67 |
| 5:FA:73:SER:HB3 | 5:FA:101:THR:HG21 | 1.77 | 0.67 |
| 1:A:264:GLN:OE1 | 1:GE:38:ASN:ND2 | 2.26 | 0.67 |
| 2:GF:236:THR:HG23 | 2:GF:367:LYS:HE3 | 1.77 | 0.67 |
| 5:HC:153:LYS:O | 5:HC:154:ILE:HG13 | 1.94 | 0.67 |
| 5:HC:360:THR:HA | 5:HC:366:PRO:HB3 | 1.77 | 0.67 |
| 7:HH:188:GLN:HG3 | 7:HJ:192:GLN:HB2 | 1.75 | 0.67 |
| 5:J:151:ILE:HD12 | 5:J:152:ASP:N | 2.10 | 0.67 |
| 1:Y:595:ILE:HG22 | 1:Y:602:ILE:HA | 1.77 | 0.67 |
| 13:YA:81[F]:ARG:NH2 | 13:YA:101[F]:GLY:HA2 | 2.09 | 0.67 |
| 14:YE:260[E]:ASP:OD1 | 14:YE:262[E]:SER:N | 2.27 | 0.67 |
| 14:YF:19[A]:SER:H | 14:YF:22[A]:ALA:HB3 | 1.60 | 0.67 |
| 14:YF:260[D]:ASP:OD1 | 14:YF:262[D]:SER:N | 2.28 | 0.67 |
| 2:Z:344:THR:OG1 | 2:Z:347:GLU:OE1 | 2.09 | 0.67 |
| 2:Z:433:ASN:ND2 | 2:Z:513:PHE:HA | 2.09 | 0.67 |
| 5:AE:102:TRP:CE3 | 5:AE:131:SER:HB2 | 2.30 | 0.66 |
| 5:AE:177:PHE:HD2 | 5:AE:230:ILE:HD11 | 1.61 | 0.66 |
| 7:AI:207:GLY:HA2 | 7:BA:193:LEU:HD11 | 1.76 | 0.66 |
| 7:AI:2:SER:O | 7:AI:6:TYR:N | 2.25 | 0.66 |
| 7:AJ:149:GLN:O | 7:AJ:153:GLY:HA2 | 1.96 | 0.66 |
| 2:BJ:926:PRO:HG3 | 2:BJ:969:TYR:CE2 | 2.30 | 0.66 |
| 5:CF:200:LEU:HD23 | 5:CF:210:SER:HA | 1.76 | 0.66 |
| 5:CH:102:TRP:CE3 | 5:CH:131:SER:HB2 | 2.30 | 0.66 |
| 5:CH:177:PHE:HD2 | 5:CH:230:ILE:HD11 | 1.60 | 0.66 |
| 1:EA:66:TYR:CE1 | 1:EB:21:PHE:HB2 | 2.27 | 0.66 |
| 12:DJ:211:HIS:HE1 | 12:GC:168:ALA:N | 1.93 | 0.66 |
| 12:GC:177:TRP:HZ3 | 12:GC:220:SER:HB3 | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GE:243:ILE:HD11 | 1:GE:252:LEU:HB3 | 1.75 | 0.66 |
| 2:GF:770:ILE:HG22 | 2:GF:842:VAL:H | 1.59 | 0.66 |
| 5:HD:130:PHE:HB3 | 5:HD:151:ILE:HG22 | 1.76 | 0.66 |
| 5:HD:263:ILE:HG22 | 5:HD:381:ILE:HB | 1.76 | 0.66 |
| 5:HD:322:GLY:N | 5:HD:358:VAL:O | 2.29 | 0.66 |
| 5:HC:551:ILE:HD13 | 5:HD:565:ILE:HD13 | 1.77 | 0.66 |
| 8:FI:43:ALA:HB1 | 8:IB:138:GLY:HA3 | 1.77 | 0.66 |
| 13:YA:408[F]:GLY:N | 13:YA:410[F]:GLU:OE2 | 2.28 | 0.66 |
| 13:YB:76[E]:PRO:HB3 | 13:YB:98[E]:GLY:CA | 2.25 | 0.66 |
| 13:YA:403[E]:PHE:HB3 | 13:YC:399[E]:HIS:CD2 | 2.30 | 0.66 |
| 14:YD:19[E]:SER:H | 14:YD:22[E]:ALA:HB3 | 1.60 | 0.66 |
| 14:YD:260[A]:ASP:OD1 | 14:YD:262[A]:SER:N | 2.27 | 0.66 |
| 2:Z:389:ASN:HB3 | 2:Z:392:THR:HG22 | 1.77 | 0.66 |
| 2:Z:539:LEU:HB3 | 2:Z:541:TYR:H | 1.60 | 0.66 |
| 5:AE:73:SER:HB3 | 5:AE:101:THR:HG21 | 1.76 | 0.66 |
| 5:AE:194:LYS:HB2 | 5:AE:243:GLN:HB2 | 1.75 | 0.66 |
| 6:AF:11:ILE:HA | 6:AH:7:LYS:HD3 | 1.77 | 0.66 |
| 7:AJ:41:PRO:O | 7:AJ:45:ASN:ND2 | 2.27 | 0.66 |
| 3:CA:47:TRP:CH2 | 3:CA:58:PRO:HB3 | 2.29 | 0.66 |
| 4:CC:168:PHE:HA | 4:CD:163:SER:HB3 | 1.76 | 0.66 |
| 5:CH:361:ASP:HB3 | 7:HH:472:ARG:NH2 | 2.10 | 0.66 |
| 7:DC:193:LEU:HD13 | 7:DD:206:GLU:HG3 | 1.76 | 0.66 |
| 12:BG:211:HIS:HE1 | 12:DJ:168:ALA:N | 1.93 | 0.66 |
| 1:EA:553:VAL:N | 1:EA:593:GLY:O | 2.21 | 0.66 |
| 2:EC:539:LEU:HB3 | 2:EC:541:TYR:H | 1.60 | 0.66 |
| 2:EC:990:MET:HG3 | 2:EC:992:PRO:HD3 | 1.78 | 0.66 |
| 5:FA:344:VAL:HG12 | 5:FA:349:TRP:HB3 | 1.77 | 0.66 |
| 5:FA:322:GLY:N | 5:FA:358:VAL:O | 2.28 | 0.66 |
| 7:FE:207:GLY:HA2 | 7:FG:193:LEU:HD11 | 1.78 | 0.66 |
| 7:FE:330:ARG:NH2 | 7:FE:336:GLU:OE2 | 2.27 | 0.66 |
| 1:GD:417:LYS:HA | 1:GD:650:TYR:O | 1.95 | 0.66 |
| 5:HB:200:LEU:HD23 | 5:HB:210:SER:HA | 1.76 | 0.66 |
| 5:HB:234:GLN:HE22 | 7:HJ:9:VAL:HG21 | 1.61 | 0.66 |
| 5:HD:312:ARG:O | 5:HD:382:ASN:N | 2.25 | 0.66 |
| 7:HH:297:TYR:N | 7:HJ:290:GLN:O | 2.26 | 0.66 |
| 5:K:130:PHE:HB3 | 5:K:151:ILE:HG22 | 1.76 | 0.66 |
| 5:K:338:ASP:HB3 | 5:K:349:TRP:CD1 | 2.29 | 0.66 |
| 7:O:447:HIS:HD2 | 7:P:447:HIS:CD2 | 2.13 | 0.66 |
| 12:W:119:ASN:O | 12:W:122:GLY:N | 2.29 | 0.66 |
| 13:YA:47[A]:ILE:HG23 | 14:YD:123[A]:PRO:HG3 | 1.78 | 0.66 |
| 13:YC:81[A]:ARG:NH2 | 13:YC:101[A]:GLY:HA2 | 2.10 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:19[B]:SER:H | 14:YE:22[B]:ALA:HB3 | 1.60 | 0.66 |
| 14:YF:288[E]:TYR:OH | 14:YF:371[E]:LYS:NZ | 2.27 | 0.66 |
| 14:YF:288[C]:TYR:OH | 14:YF:371[C]:LYS:NZ | 2.27 | 0.66 |
| 2:Z:251:ASP:OD2 | 2:Z:252:LYS:NZ | 2.26 | 0.66 |
| 1:A:417:LYS:HA | 1:A:650:TYR:O | 1.95 | 0.66 |
| 5:AC:193:VAL:HG13 | 5:AC:199:GLU:HB3 | 1.78 | 0.66 |
| 5:AC:407:TYR:CE1 | 5:AE:407:TYR:HB2 | 2.29 | 0.66 |
| 5:AD:151:ILE:HD12 | 5:AD:152:ASP:N | 2.10 | 0.66 |
| 5:AD:360:THR:HA | 5:AD:366:PRO:HB3 | 1.77 | 0.66 |
| 7:AI:351:ALA:O | 7:AI:520:ASN:ND2 | 2.29 | 0.66 |
| 7:BA:334:GLN:HG3 | 7:BA:337:ILE:HD12 | 1.78 | 0.66 |
| 12:BG:125:ILE:HA | 12:BG:162:PHE:HB3 | 1.78 | 0.66 |
| 1:BH:195:ASN:OD1 | 1:BH:352:ARG:NH1 | 2.23 | 0.66 |
| 1:BH:522:LYS:HA | 1:BH:534:VAL:HG23 | 1.78 | 0.66 |
| 5:CG:151:ILE:HD12 | 5:CG:152:ASP:N | 2.10 | 0.66 |
| 2:C:87:GLN:NE2 | 3:D:158:GLY:HA2 | 2.10 | 0.66 |
| 7:FG:325:TYR:HD1 | 7:FG:330:ARG:HA | 1.61 | 0.66 |
| 1:GD:522:LYS:HA | 1:GD:534:VAL:HG23 | 1.78 | 0.66 |
| 2:GF:332:SER:OG | 2:GF:333:ASN:O | 2.11 | 0.66 |
| 2:GF:58:ASN:OD1 | 2:GF:60:GLY:N | 2.23 | 0.66 |
| 5:HC:111:ALA:HB2 | 5:HC:117:ILE:HG23 | 1.78 | 0.66 |
| 5:HC:305:ASN:ND2 | 5:HD:255:ARG:O | 2.28 | 0.66 |
| 5:HD:62:ALA:HB1 | 5:HD:82:PRO:HG3 | 1.76 | 0.66 |
| 5:I:193:VAL:HG13 | 5:I:199:GLU:HB3 | 1.78 | 0.66 |
| 12:IF:119:ASN:O | 12:IF:122:GLY:N | 2.29 | 0.66 |
| 6:L:60:HIS:NE2 | 6:N:28:ASP:OD2 | 2.29 | 0.66 |
| 12:W:177:TRP:HZ3 | 12:W:220:SER:HB3 | 1.60 | 0.66 |
| 13:YC:408[C]:GLY:N | 13:YC:410[C]:GLU:OE2 | 2.27 | 0.66 |
| 14:YD:211[E]:MET:HE1 | 14:YD:231[E]:ALA:HB2 | 1.77 | 0.66 |
| 14:YD:288[C]:TYR:OH | 14:YD:371[C]:LYS:NZ | 2.27 | 0.66 |
| 14:YE:36[D]:THR:HG22 | 14:YE:37[D]:THR:HG23 | 1.75 | 0.66 |
| 14:YF:211[B]:MET:HE1 | 14:YF:231[B]:ALA:HB2 | 1.75 | 0.66 |
| 14:YF:260[C]:ASP:OD1 | 14:YF:262[C]:SER:N | 2.28 | 0.66 |
| 2:Z:332:SER:OG | 2:Z:333:ASN:O | 2.11 | 0.66 |
| 5:AC:200:LEU:HD23 | 5:AC:210:SER:HA | 1.76 | 0.66 |
| 5:AC:234:GLN:HE22 | 7:BA:9:VAL:HG21 | 1.60 | 0.66 |
| 5:AD:251:VAL:O | 5:AE:161:ASN:ND2 | 2.28 | 0.66 |
| 7:AI:447:HIS:HD2 | 7:AJ:447:HIS:CD2 | 2.13 | 0.66 |
| 12:BG:177:TRP:HZ3 | 12:BG:220:SER:HB3 | 1.60 | 0.66 |
| 2:BJ:777:LEU:HD23 | 2:BJ:809:TRP:CG | 2.30 | 0.66 |
| 1:B:338:ARG:NH1 | 2:C:738:LYS:O | 2.22 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:752:TYR:OH | 2:C:878:ASP:OD2 | 2.11 | 0.66 |
| 5:CF:264:ARG:HB3 | 5:CH:326:MET:CE | 2.26 | 0.66 |
| 7:DC:149:GLN:O | 7:DC:153:GLY:HA2 | 1.95 | 0.66 |
| 12:DJ:147:ASN:OD1 | 12:DJ:148:ILE:N | 2.27 | 0.66 |
| 2:EC:340:PRO:HA | 2:EC:345:TYR:CE1 | 2.30 | 0.66 |
| 5:EJ:151:ILE:HD12 | 5:EJ:152:ASP:N | 2.10 | 0.66 |
| 5:EJ:170:GLU:HA | 5:EJ:238:ILE:HG13 | 1.76 | 0.66 |
| 5:FA:102:TRP:CE3 | 5:FA:131:SER:HB2 | 2.30 | 0.66 |
| 5:EJ:569:TYR:OH | 5:FA:571:GLU:OE2 | 2.11 | 0.66 |
| 7:FE:212:PRO:HB3 | 7:FF:199:VAL:HA | 1.78 | 0.66 |
| 7:FF:497:ASN:H | 7:FF:500:TYR:HB2 | 1.61 | 0.66 |
| 11:GB:129:ASN:HB2 | 11:GB:132:VAL:HG12 | 1.77 | 0.66 |
| 12:GC:119:ASN:O | 12:GC:122:GLY:N | 2.29 | 0.66 |
| 3:E:229:LEU:HD23 | 2:GF:509:TYR:HB3 | 1.77 | 0.66 |
| 2:GF:87:GLN:NE2 | 3:GG:158:GLY:HA2 | 2.11 | 0.66 |
| 4:G:275:ALA:O | 4:H:282:GLN:NE2 | 2.27 | 0.66 |
| 5:HC:326:MET:HE1 | 5:HD:264:ARG:N | 2.11 | 0.66 |
| 7:HH:141:VAL:HG22 | 7:HI:139:ASN:HB2 | 1.77 | 0.66 |
| 9:IC:59:ASP:HA | 9:IC:62:PHE:HB3 | 1.77 | 0.66 |
| 5:J:111:ALA:HB2 | 5:J:117:ILE:HG23 | 1.78 | 0.66 |
| 5:K:322:GLY:N | 5:K:358:VAL:O | 2.29 | 0.66 |
| 5:K:344:VAL:HG12 | 5:K:349:TRP:HB3 | 1.77 | 0.66 |
| 5:K:72:THR:OG1 | 5:K:101:THR:O | 2.11 | 0.66 |
| 7:O:212:PRO:HB3 | 7:P:199:VAL:HA | 1.78 | 0.66 |
| 7:Q:334:GLN:HG3 | 7:Q:337:ILE:HD12 | 1.78 | 0.66 |
| 11:V:178:ASN:N | 14:YD:217[A]:SER:O | 2.27 | 0.66 |
| 13:YC:408[F]:GLY:N | 13:YC:410[F]:GLU:OE2 | 2.27 | 0.66 |
| 13:YA:24[B]:LEU:HD23 | 14:YD:259[B]:LEU:HD22 | 1.78 | 0.66 |
| 14:YE:211[E]:MET:HE1 | 14:YE:231[E]:ALA:HB2 | 1.77 | 0.66 |
| 14:YF:211[C]:MET:HE1 | 14:YF:231[C]:ALA:HB2 | 1.77 | 0.66 |
| 5:AD:153:LYS:O | 5:AD:154:ILE:HG13 | 1.94 | 0.66 |
| 5:AC:577:ASN:ND2 | 5:AD:529:ASN:OD1 | 2.23 | 0.66 |
| 7:AI:20:PRO:HG3 | 7:AI:29:ILE:HG13 | 1.76 | 0.66 |
| 2:BJ:118:LEU:HD21 | 2:BJ:122:PHE:HD2 | 1.59 | 0.66 |
| 2:BJ:87:GLN:NE2 | 3:CA:158:GLY:HA2 | 2.11 | 0.66 |
| 2:C:770:ILE:HG22 | 2:C:842:VAL:H | 1.58 | 0.66 |
| 5:CG:507:ASP:OD1 | 5:CG:511:ASN:N | 2.22 | 0.66 |
| 5:CH:322:GLY:N | 5:CH:358:VAL:O | 2.28 | 0.66 |
| 6:CI:16:ASP:OD2 | 6:CI:45:LYS:NZ | 2.29 | 0.66 |
| 7:DB:351:ALA:O | 7:DB:520:ASN:ND2 | 2.28 | 0.66 |
| 7:DC:146:SER:H | 7:DC:149:GLN:HB2 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:448:ALA:N | 7:DC:485:ASN:OD1 | 2.28 | 0.66 |
| 3:ED:54:VAL:HG23 | 3:EE:5:SER:HA | 1.77 | 0.66 |
| 5:EI:164:ARG:HG3 | 5:EI:245:GLU:HG2 | 1.78 | 0.66 |
| 5:EJ:312:ARG:HG2 | 5:EJ:317:LEU:HA | 1.78 | 0.66 |
| 5:FA:491:ASN:HD22 | 5:FA:496:ASP:HB2 | 1.61 | 0.66 |
| 7:FG:375:TYR:OH | 7:FG:391:GLY:O | 2.14 | 0.66 |
| 2:GF:926:PRO:HG3 | 2:GF:969:TYR:CE2 | 2.30 | 0.66 |
| 2:GF:990:MET:HG3 | 2:GF:992:PRO:HD3 | 1.78 | 0.66 |
| 4:GI:282:GLN:NE2 | 4:HA:275:ALA:O | 2.28 | 0.66 |
| 7:HJ:334:GLN:HG3 | 7:HJ:337:ILE:HD12 | 1.78 | 0.66 |
| 7:HI:486:ASP:HB2 | 7:HJ:444:TYR:HB2 | 1.76 | 0.66 |
| 5:K:316:ILE:HG22 | 5:K:318:GLN:HG3 | 1.78 | 0.66 |
| 6:M:39:THR:OG1 | 6:M:42:GLN:OE1 | 2.14 | 0.66 |
| 7:O:289:GLN:HA | 7:P:287:VAL:HA | 1.78 | 0.66 |
| 13:YA:408[B]:GLY:N | 13:YA:410[B]:GLU:OE2 | 2.28 | 0.66 |
| 13:YA:514[F]:VAL:O | 13:YC:522[F]:VAL:HA | 1.96 | 0.66 |
| 13:YB:408[B]:GLY:N | 13:YB:410[B]:GLU:OE2 | 2.28 | 0.66 |
| 13:YB:408[C]:GLY:N | 13:YB:410[C]:GLU:OE2 | 2.27 | 0.66 |
| 13:YB:408[D]:GLY:N | 13:YB:410[D]:GLU:OE2 | 2.28 | 0.66 |
| 13:YB:408[F]:GLY:N | 13:YB:410[F]:GLU:OE2 | 2.28 | 0.66 |
| 13:YC:408[B]:GLY:N | 13:YC:410[B]:GLU:OE2 | 2.28 | 0.66 |
| 13:YC:408[D]:GLY:N | 13:YC:410[D]:GLU:OE2 | 2.28 | 0.66 |
| 14:YD:288[B]:TYR:OH | 14:YD:371[B]:LYS:NZ | 2.27 | 0.66 |
| 14:YE:215[E]:GLU:OE1 | 14:YF:100[E]:LYS:NZ | 2.29 | 0.66 |
| 14:YE:288[F]:TYR:OH | 14:YE:371[F]:LYS:NZ | 2.27 | 0.66 |
| 14:YF:19[F]:SER:H | 14:YF:22[F]:ALA:HB3 | 1.61 | 0.66 |
| 2:Z:584:GLY:HA2 | 2:Z:600:PHE:HB3 | 1.78 | 0.66 |
| 5:AC:264:ARG:HB3 | 5:AE:326:MET:CE | 2.26 | 0.66 |
| 7:AI:170:ILE:HD13 | 7:AJ:172:LEU:HD22 | 1.77 | 0.66 |
| 2:BJ:154:SER:OG | 2:BJ:156:SER:OG | 2.13 | 0.66 |
| 2:BJ:81:ARG:HD2 | 2:BJ:94:TRP:HB3 | 1.78 | 0.66 |
| 4:CC:163:SER:HB3 | 4:CE:168:PHE:HA | 1.78 | 0.66 |
| 5:CG:119:GLY:H | 5:CG:142:ARG:HH22 | 1.44 | 0.66 |
| 7:DC:41:PRO:O | 7:DC:45:ASN:ND2 | 2.27 | 0.66 |
| 12:DJ:125:ILE:HA | 12:DJ:162:PHE:HB3 | 1.78 | 0.66 |
| 2:EC:118:LEU:HD21 | 2:EC:122:PHE:HD2 | 1.59 | 0.66 |
| 2:EC:584:GLY:HA2 | 2:EC:600:PHE:HB3 | 1.78 | 0.66 |
| 5:FA:263:ILE:HG22 | 5:FA:381:ILE:HB | 1.76 | 0.66 |
| 5:FA:318:GLN:HB3 | 6:FC:4:LEU:HG | 1.76 | 0.66 |
| 11:GB:123:LEU:HD12 | 11:GB:135:ASP:HA | 1.77 | 0.66 |
| 1:GD:99:LEU:HG | 1:GD:211:ARG:HH12 | 1.59 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:90:VAL:O | 1:GD:94:GLN:N | 2.26 | 0.66 |
| 2:GF:539:LEU:HB3 | 2:GF:541:TYR:H | 1.60 | 0.66 |
| 2:GF:81:ARG:HD2 | 2:GF:94:TRP:HB3 | 1.77 | 0.66 |
| 5:HD:73:SER:HB3 | 5:HD:101:THR:HG21 | 1.77 | 0.66 |
| 5:HD:102:TRP:CE3 | 5:HD:131:SER:HB2 | 2.30 | 0.66 |
| 5:HD:491:ASN:HD22 | 5:HD:496:ASP:HB2 | 1.61 | 0.66 |
| 7:HH:351:ALA:O | 7:HH:520:ASN:ND2 | 2.29 | 0.66 |
| 7:HH:41:PRO:O | 7:HH:45:ASN:ND2 | 2.29 | 0.66 |
| 7:HJ:325:TYR:HD1 | 7:HJ:330:ARG:HA | 1.61 | 0.66 |
| 7:HJ:375:TYR:OH | 7:HJ:391:GLY:O | 2.14 | 0.66 |
| 5:J:312:ARG:HG2 | 5:J:317:LEU:HA | 1.78 | 0.66 |
| 5:J:251:VAL:O | 5:K:161:ASN:ND2 | 2.28 | 0.66 |
| 5:K:175:THR:O | 5:K:232:LEU:N | 2.26 | 0.66 |
| 5:K:177:PHE:HD2 | 5:K:230:ILE:HD11 | 1.60 | 0.66 |
| 5:K:263:ILE:HG22 | 5:K:381:ILE:HB | 1.76 | 0.66 |
| 5:K:73:SER:HB3 | 5:K:101:THR:HG21 | 1.77 | 0.66 |
| 6:L:39:THR:OG1 | 6:L:42:GLN:OE1 | 2.14 | 0.66 |
| 7:P:149:GLN:O | 7:P:153:GLY:HA2 | 1.95 | 0.66 |
| 7:P:512:THR:HA | 7:Q:442:MET:HA | 1.78 | 0.66 |
| 7:Q:177:ALA:HB3 | 7:Q:178:PRO:HD3 | 1.78 | 0.66 |
| 11:V:123:LEU:HD12 | 11:V:135:ASP:HA | 1.77 | 0.66 |
| 12:W:125:ILE:HA | 12:W:162:PHE:HB3 | 1.78 | 0.66 |
| 1:X:99:LEU:HG | 1:X:211:ARG:HH12 | 1.59 | 0.66 |
| 13:YA:403[A]:PHE:HB3 | 13:YC:399[A]:HIS:CD2 | 2.30 | 0.66 |
| 13:YB:61[A]:ILE:HA | 13:YC:76[A]:PRO:CA | 2.24 | 0.66 |
| 13:YA:514[E]:VAL:O | 13:YC:522[E]:VAL:HA | 1.96 | 0.66 |
| 14:YE:211[D]:MET:HE1 | 14:YE:231[D]:ALA:HB2 | 1.75 | 0.66 |
| 11:V:178:ASN:N | 14:YE:217[E]:SER:O | 2.27 | 0.66 |
| 14:YE:19[E]:SER:H | 14:YE:22[E]:ALA:HB3 | 1.60 | 0.66 |
| 14:YE:366[F]:THR:O | 14:YE:369[F]:PRO:HD3 | 1.96 | 0.66 |
| 13:YC:47[B]:ILE:HG23 | 14:YF:123[B]:PRO:HG3 | 1.78 | 0.66 |
| 2:Z:312:THR:HB | 2:Z:319:TYR:HB2 | 1.75 | 0.66 |
| 5:AC:164:ARG:HG3 | 5:AC:245:GLU:HG2 | 1.78 | 0.66 |
| 5:AE:221:GLU:OE2 | 5:AE:233:ARG:NH2 | 2.29 | 0.66 |
| 7:AJ:233:GLN:HE21 | 7:AJ:237:ASN:HD21 | 1.44 | 0.66 |
| 10:BE:214:ARG:NH1 | 12:BG:246:ARG:HH12 | 1.93 | 0.66 |
| 12:BG:9:ASN:O | 12:BG:13:ASN:ND2 | 2.28 | 0.66 |
| 1:BH:417:LYS:HA | 1:BH:650:TYR:O | 1.95 | 0.66 |
| 1:BI:338:ARG:NH1 | 2:BJ:738:LYS:O | 2.23 | 0.66 |
| 2:BJ:990:MET:HG3 | 2:BJ:992:PRO:HD3 | 1.78 | 0.66 |
| 1:B:230:ILE:HD13 | 2:C:691:ARG:HG3 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:981:GLN:N | 2:C:981:GLN:OE1 | 2.29 | 0.66 |
| 5:EI:241:THR:HG21 | 5:FA:200:LEU:HD13 | 1.76 | 0.66 |
| 7:FE:102:THR:HG22 | 7:FE:105:GLU:HG3 | 1.76 | 0.66 |
| 7:FF:386:ASN:OD1 | 7:FF:389:ASN:N | 2.29 | 0.66 |
| 1:EA:84:ASN:ND2 | 11:GB:14:LYS:O | 2.27 | 0.66 |
| 2:GF:118:LEU:HD21 | 2:GF:122:PHE:HD2 | 1.59 | 0.66 |
| 2:GF:584:GLY:HA2 | 2:GF:600:PHE:HB3 | 1.78 | 0.66 |
| 5:HC:312:ARG:HG2 | 5:HC:317:LEU:HA | 1.78 | 0.66 |
| 5:HC:31:ASP:O | 5:HC:35:TYR:N | 2.26 | 0.66 |
| 5:J:320:LEU:HD23 | 5:J:358:VAL:HG23 | 1.76 | 0.66 |
| 7:O:449:GLY:HA2 | 7:P:484:THR:HG22 | 1.78 | 0.66 |
| 7:P:233:GLN:HE21 | 7:P:237:ASN:HD21 | 1.44 | 0.66 |
| 13:YA:408[A]:GLY:N | 13:YA:410[A]:GLU:OE2 | 2.28 | 0.66 |
| 13:YA:408[E]:GLY:N | 13:YA:410[E]:GLU:OE2 | 2.28 | 0.66 |
| 14:YD:100[C]:LYS:NZ | 14:YF:215[C]:GLU:OE1 | 2.29 | 0.66 |
| 14:YD:19[D]:SER:H | 14:YD:22[D]:ALA:HB3 | 1.61 | 0.66 |
| 14:YE:366[E]:THR:O | 14:YE:369[E]:PRO:HD3 | 1.96 | 0.66 |
| 14:YF:19[D]:SER:H | 14:YF:22[D]:ALA:HB3 | 1.60 | 0.66 |
| 14:YF:366[D]:THR:O | 14:YF:369[D]:PRO:HD3 | 1.96 | 0.66 |
| 2:Z:3:VAL:O | 2:Z:90:GLU:N | 2.26 | 0.66 |
| 1:A:236:PHE:CE2 | 1:A:270:ILE:HD11 | 2.30 | 0.66 |
| 5:AD:119:GLY:H | 5:AD:142:ARG:HH22 | 1.44 | 0.66 |
| 5:AE:312:ARG:O | 5:AE:382:ASN:N | 2.25 | 0.66 |
| 7:AI:41:PRO:O | 7:AI:45:ASN:ND2 | 2.29 | 0.66 |
| 1:B:543:THR:HG21 | 1:B:551:GLY:HA3 | 1.78 | 0.66 |
| 2:C:236:THR:HG23 | 2:C:367:LYS:HE3 | 1.77 | 0.66 |
| 3:CB:51:GLU:OE2 | 3:CB:270:ARG:NH2 | 2.29 | 0.66 |
| 5:CF:193:VAL:HG13 | 5:CF:199:GLU:HB3 | 1.78 | 0.66 |
| 5:CH:221:GLU:OE2 | 5:CH:233:ARG:NH2 | 2.29 | 0.66 |
| 5:CH:73:SER:HB3 | 5:CH:101:THR:HG21 | 1.76 | 0.66 |
| 5:EJ:327:PRO:HG3 | 5:FA:264:ARG:HD3 | 1.77 | 0.66 |
| 5:FA:177:PHE:HD2 | 5:FA:230:ILE:HD11 | 1.60 | 0.66 |
| 5:FA:270:LEU:HG | 6:FD:108:LEU:HD21 | 1.78 | 0.66 |
| 4:GI:64:THR:HA | 4:GJ:84:ARG:HE | 1.59 | 0.66 |
| 2:GF:940:GLY:O | 5:HB:21:LYS:NZ | 2.29 | 0.66 |
| 5:HB:312:ARG:HB2 | 5:HB:382:ASN:HB2 | 1.78 | 0.66 |
| 6:HG:39:THR:OG1 | 6:HG:42:GLN:OE1 | 2.14 | 0.66 |
| 5:HD:196:ARG:NH1 | 7:HI:5:THR:O | 2.29 | 0.66 |
| 9:IC:10:ASP:OD1 | 9:IC:11:ILE:N | 2.28 | 0.66 |
| 5:J:170:GLU:HA | 5:J:238:ILE:HG13 | 1.76 | 0.66 |
| 7:O:20:PRO:HG3 | 7:O:29:ILE:HG13 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:41:PRO:O | 7:O:45:ASN:ND2 | 2.29 | 0.66 |
| 7:O:170:ILE:HD13 | 7:P:172:LEU:HD22 | 1.77 | 0.66 |
| 7:P:193:LEU:HD13 | 7:Q:206:GLU:HG3 | 1.76 | 0.66 |
| 7:O:498:SER:O | 7:Q:422:LYS:NZ | 2.29 | 0.66 |
| 13:YA:408[D]:GLY:N | 13:YA:410[D]:GLU:OE2 | 2.28 | 0.66 |
| 13:YA:514[B]:VAL:O | 13:YC:522[B]:VAL:HA | 1.96 | 0.66 |
| 13:YC:408[A]:GLY:N | 13:YC:410[A]:GLU:OE2 | 2.28 | 0.66 |
| 14:YD:100[A]:LYS:NZ | 14:YF:215[A]:GLU:OE1 | 2.28 | 0.66 |
| 14:YD:19[A]:SER:H | 14:YD:22[A]:ALA:HB3 | 1.60 | 0.66 |
| 2:Z:118:LEU:HD21 | 2:Z:122:PHE:HD2 | 1.59 | 0.66 |
| 5:AD:223:VAL:HB | 5:AD:224:PRO:HD3 | 1.78 | 0.66 |
| 5:AD:237:ASN:OD1 | 5:AD:238:ILE:N | 2.29 | 0.66 |
| 7:BA:177:ALA:HB3 | 7:BA:178:PRO:HD3 | 1.78 | 0.66 |
| 7:BA:325:TYR:HD1 | 7:BA:330:ARG:HA | 1.61 | 0.66 |
| 11:BF:129:ASN:HB2 | 11:BF:132:VAL:HG12 | 1.77 | 0.66 |
| 2:BJ:584:GLY:HA2 | 2:BJ:600:PHE:HB3 | 1.78 | 0.66 |
| 2:C:118:LEU:HD21 | 2:C:122:PHE:HD2 | 1.59 | 0.66 |
| 2:C:926:PRO:HG3 | 2:C:969:TYR:CE2 | 2.30 | 0.66 |
| 4:CC:64:THR:HA | 4:CD:84:ARG:HE | 1.60 | 0.66 |
| 6:CI:13:ARG:HD2 | 6:DA:10:VAL:HA | 1.78 | 0.66 |
| 6:CJ:39:THR:OG1 | 6:CJ:42:GLN:OE1 | 2.14 | 0.66 |
| 7:DC:130:GLU:HG2 | 7:DD:139:ASN:HD21 | 1.61 | 0.66 |
| 3:EE:170:PRO:HB3 | 3:EE:188:TRP:CD1 | 2.30 | 0.66 |
| 5:EJ:119:GLY:H | 5:EJ:142:ARG:HH22 | 1.44 | 0.66 |
| 5:FA:85:THR:HB | 5:FA:137:TYR:CE2 | 2.31 | 0.66 |
| 7:FF:150:ALA:HB3 | 7:FF:168:LEU:HD13 | 1.78 | 0.66 |
| 1:GE:361:GLN:HG2 | 1:GE:455:PHE:CE2 | 2.31 | 0.66 |
| 7:HH:330:ARG:NH2 | 7:HH:336:GLU:OE2 | 2.27 | 0.66 |
| 7:HI:130:GLU:HG2 | 7:HJ:139:ASN:HD21 | 1.61 | 0.66 |
| 11:IE:123:LEU:HD12 | 11:IE:135:ASP:HA | 1.77 | 0.66 |
| 12:IF:9:ASN:O | 12:IF:13:ASN:ND2 | 2.28 | 0.66 |
| 7:O:102:THR:HG22 | 7:O:105:GLU:HG3 | 1.76 | 0.66 |
| 7:O:351:ALA:O | 7:O:520:ASN:ND2 | 2.28 | 0.66 |
| 7:Q:375:TYR:OH | 7:Q:391:GLY:O | 2.14 | 0.66 |
| 9:T:10:ASP:OD1 | 9:T:11:ILE:N | 2.28 | 0.66 |
| 1:Y:543:THR:HG21 | 1:Y:551:GLY:HA3 | 1.78 | 0.66 |
| 13:YB:408[E]:GLY:N | 13:YB:410[E]:GLU:OE2 | 2.28 | 0.66 |
| 14:YD:19[B]:SER:H | 14:YD:22[B]:ALA:HB3 | 1.60 | 0.66 |
| 14:YD:366[B]:THR:O | 14:YD:369[B]:PRO:HD3 | 1.96 | 0.66 |
| 14:YF:19[C]:SER:H | 14:YF:22[C]:ALA:HB3 | 1.60 | 0.66 |
| 14:YF:288[D]:TYR:OH | 14:YF:371[D]:LYS:NZ | 2.27 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:236:THR:HG23 | 2:Z:367:LYS:HE3 | 1.77 | 0.66 |
| 2:Z:777:LEU:HD23 | 2:Z:809:TRP:CG | 2.30 | 0.66 |
| 1:A:99:LEU:HG | 1:A:211:ARG:HH12 | 1.59 | 0.66 |
| 5:AD:170:GLU:HA | 5:AD:238:ILE:HG13 | 1.76 | 0.66 |
| 5:AD:329:PHE:HB3 | 5:AD:332:VAL:HB | 1.78 | 0.66 |
| 5:AE:322:GLY:N | 5:AE:358:VAL:O | 2.29 | 0.66 |
| 6:AG:39:THR:OG1 | 6:AG:42:GLN:OE1 | 2.14 | 0.66 |
| 7:AI:141:VAL:HG22 | 7:AJ:139:ASN:HB2 | 1.77 | 0.66 |
| 7:AI:211:SER:N | 7:AI:214:THR:OG1 | 2.28 | 0.66 |
| 7:AJ:512:THR:HA | 7:BA:442:MET:HA | 1.78 | 0.66 |
| 2:C:332:SER:OG | 2:C:333:ASN:O | 2.11 | 0.66 |
| 5:CF:407:TYR:CE1 | 5:CH:407:TYR:HB2 | 2.30 | 0.66 |
| 7:DC:512:THR:HA | 7:DD:442:MET:HA | 1.78 | 0.66 |
| 7:DD:375:TYR:OH | 7:DD:391:GLY:O | 2.14 | 0.66 |
| 8:DF:43:ALA:HB1 | 8:FI:138:GLY:HA3 | 1.76 | 0.66 |
| 2:EC:389:ASN:HB3 | 2:EC:392:THR:HG22 | 1.77 | 0.66 |
| 4:F:163:SER:HB3 | 4:H:168:PHE:HA | 1.78 | 0.66 |
| 5:EI:24:ILE:HG13 | 5:FA:7:ILE:HD11 | 1.78 | 0.66 |
| 6:FB:13:ARG:HD2 | 6:FD:10:VAL:HA | 1.78 | 0.66 |
| 6:FB:218:THR:HB | 7:HI:205:ARG:HH12 | 1.61 | 0.66 |
| 12:GC:9:ASN:O | 12:GC:13:ASN:ND2 | 2.28 | 0.66 |
| 1:GE:38:ASN:OD1 | 1:GE:39:GLY:N | 2.27 | 0.66 |
| 7:HH:498:SER:O | 7:HJ:422:LYS:NZ | 2.29 | 0.66 |
| 7:HI:146:SER:H | 7:HI:149:GLN:HB2 | 1.61 | 0.66 |
| 7:HI:150:ALA:HB3 | 7:HI:168:LEU:HD13 | 1.78 | 0.66 |
| 5:I:312:ARG:HB2 | 5:I:382:ASN:HB2 | 1.78 | 0.66 |
| 7:P:150:ALA:HB3 | 7:P:168:LEU:HD13 | 1.78 | 0.66 |
| 7:P:386:ASN:OD1 | 7:P:389:ASN:N | 2.29 | 0.66 |
| 7:P:497:ASN:H | 7:P:500:TYR:HB2 | 1.60 | 0.66 |
| 13:YA:551[F]:THR:HG22 | 13:YC:558[F]:SER:HB3 | 1.78 | 0.66 |
| 11:DI:178:ASN:N | 14:YD:217[D]:SER:O | 2.27 | 0.66 |
| 13:YA:24[C]:LEU:HD23 | 14:YD:259[C]:LEU:HD22 | 1.78 | 0.66 |
| 14:YD:366[A]:THR:O | 14:YD:369[A]:PRO:HD3 | 1.96 | 0.66 |
| 14:YE:19[F]:SER:H | 14:YE:22[F]:ALA:HB3 | 1.61 | 0.66 |
| 14:YF:366[C]:THR:O | 14:YF:369[C]:PRO:HD3 | 1.96 | 0.66 |
| 2:Z:926:PRO:HG3 | 2:Z:969:TYR:CE2 | 2.30 | 0.66 |
| 9:BD:98:VAL:N | 9:BD:103:THR:O | 2.26 | 0.65 |
| 9:BD:10:ASP:OD1 | 9:BD:11:ILE:N | 2.28 | 0.65 |
| 9:BD:59:ASP:HA | 9:BD:62:PHE:HB3 | 1.77 | 0.65 |
| 1:BH:236:PHE:CE2 | 1:BH:270:ILE:HD11 | 2.30 | 0.65 |
| 2:C:584:GLY:HA2 | 2:C:600:PHE:HB3 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:134:TYR:OH | 2:C:593:GLU:HG2 | 1.97 | 0.65 |
| 2:C:777:LEU:HD23 | 2:C:809:TRP:CG | 2.30 | 0.65 |
| 3:CA:92:ARG:HB3 | 3:CA:208:ILE:HG23 | 1.77 | 0.65 |
| 7:DB:141:VAL:HG22 | 7:DC:139:ASN:HB2 | 1.76 | 0.65 |
| 7:DB:330:ARG:NH2 | 7:DB:336:GLU:OE2 | 2.27 | 0.65 |
| 7:DC:386:ASN:OD1 | 7:DC:389:ASN:N | 2.29 | 0.65 |
| 7:DD:177:ALA:HB3 | 7:DD:178:PRO:HD3 | 1.78 | 0.65 |
| 7:DD:334:GLN:HG3 | 7:DD:337:ILE:HD12 | 1.78 | 0.65 |
| 12:DJ:9:ASN:O | 12:DJ:13:ASN:ND2 | 2.28 | 0.65 |
| 5:EJ:34:TYR:OH | 5:EJ:40:GLY:O | 2.03 | 0.65 |
| 12:GC:125:ILE:HA | 12:GC:162:PHE:HB3 | 1.78 | 0.65 |
| 1:GE:543:THR:HG21 | 1:GE:551:GLY:HA3 | 1.78 | 0.65 |
| 2:GF:884:HIS:ND1 | 2:GF:885:PRO:O | 2.29 | 0.65 |
| 3:GG:92:ARG:HB3 | 3:GG:208:ILE:HG23 | 1.77 | 0.65 |
| 7:HH:102:THR:HG22 | 7:HH:105:GLU:HG3 | 1.76 | 0.65 |
| 7:HI:512:THR:HA | 7:HJ:442:MET:HA | 1.78 | 0.65 |
| 8:R:138:GLY:HA3 | 8:IA:43:ALA:CB | 2.25 | 0.65 |
| 5:J:223:VAL:HB | 5:J:224:PRO:HD3 | 1.78 | 0.65 |
| 13:YA:403[C]:PHE:HB3 | 13:YC:399[C]:HIS:CD2 | 2.30 | 0.65 |
| 13:YB:81[D]:ARG:NH2 | 13:YB:101[D]:GLY:HA2 | 2.09 | 0.65 |
| 13:YB:38[C]:GLN:OE1 | 13:YB:38[C]:GLN:N | 2.29 | 0.65 |
| 13:YA:76[A]:PRO:CA | 13:YC:61[A]:ILE:HA | 2.26 | 0.65 |
| 14:YD:215[C]:GLU:OE1 | 14:YE:100[C]:LYS:NZ | 2.29 | 0.65 |
| 14:YE:245[B]:ARG:NE | 14:YE:246[B]:ASP:OD1 | 2.25 | 0.65 |
| 11:IE:178:ASN:N | 14:YF:217[B]:SER:O | 2.28 | 0.65 |
| 1:A:506:LYS:O | 1:A:509:SER:OG | 2.11 | 0.65 |
| 4:AA:168:PHE:HA | 4:AB:163:SER:HB3 | 1.79 | 0.65 |
| 5:AC:312:ARG:HB2 | 5:AC:382:ASN:HB2 | 1.78 | 0.65 |
| 5:AE:85:THR:HB | 5:AE:137:TYR:CE2 | 2.31 | 0.65 |
| 7:AI:498:SER:O | 7:BA:422:LYS:NZ | 2.29 | 0.65 |
| 12:BG:15:ASP:CG | 12:BG:16:PHE:H | 2.00 | 0.65 |
| 1:BH:156:ASP:OD1 | 1:BH:157:LYS:N | 2.29 | 0.65 |
| 1:BI:521:ARG:O | 1:BI:533:ASP:HB2 | 1.97 | 0.65 |
| 2:BJ:134:TYR:OH | 2:BJ:593:GLU:HG2 | 1.97 | 0.65 |
| 2:C:990:MET:HG3 | 2:C:992:PRO:HD3 | 1.78 | 0.65 |
| 5:CG:170:GLU:HA | 5:CG:238:ILE:HG13 | 1.76 | 0.65 |
| 5:CG:329:PHE:HB3 | 5:CG:332:VAL:HB | 1.78 | 0.65 |
| 7:DB:176:ILE:HG12 | 7:DB:177:ALA:H | 1.61 | 0.65 |
| 9:DG:10:ASP:OD1 | 9:DG:11:ILE:N | 2.29 | 0.65 |
| 12:DJ:119:ASN:O | 12:DJ:122:GLY:N | 2.29 | 0.65 |
| 12:DJ:177:TRP:HZ3 | 12:DJ:220:SER:HB3 | 1.60 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:312:ARG:HB2 | 5:EI:382:ASN:HB2 | 1.78 | 0.65 |
| 4:F:64:THR:HA | 4:G:84:ARG:HE | 1.60 | 0.65 |
| 6:FB:16:ASP:OD2 | 6:FB:45:LYS:NZ | 2.29 | 0.65 |
| 7:FE:441:GLN:NE2 | 7:FG:509:GLY:HA3 | 2.10 | 0.65 |
| 7:FE:496:ARG:NH1 | 7:FE:501:THR:OG1 | 2.29 | 0.65 |
| 1:GE:290:ASP:OD1 | 1:GE:291:THR:N | 2.28 | 0.65 |
| 5:HB:397:ASP:O | 5:HB:401:ASP:N | 2.19 | 0.65 |
| 7:HH:211:SER:N | 7:HH:214:THR:OG1 | 2.28 | 0.65 |
| 7:HI:497:ASN:H | 7:HI:500:TYR:HB2 | 1.61 | 0.65 |
| 9:IC:98:VAL:N | 9:IC:103:THR:O | 2.26 | 0.65 |
| 12:IF:125:ILE:HA | 12:IF:162:PHE:HB3 | 1.78 | 0.65 |
| 5:J:594:THR:OG1 | 5:K:517:GLY:N | 2.27 | 0.65 |
| 5:K:85:THR:HB | 5:K:137:TYR:CE2 | 2.31 | 0.65 |
| 6:N:39:THR:OG1 | 6:N:42:GLN:OE1 | 2.14 | 0.65 |
| 7:P:146:SER:H | 7:P:149:GLN:HB2 | 1.61 | 0.65 |
| 7:P:130:GLU:HG2 | 7:Q:139:ASN:HD21 | 1.61 | 0.65 |
| 13:YA:38[D]:GLN:N | 13:YA:38[D]:GLN:OE1 | 2.29 | 0.65 |
| 13:YA:514[A]:VAL:O | 13:YC:522[A]:VAL:HA | 1.96 | 0.65 |
| 13:YA:514[C]:VAL:O | 13:YC:522[C]:VAL:HA | 1.96 | 0.65 |
| 13:YA:403[F]:PHE:HB3 | 13:YC:399[F]:HIS:CD2 | 2.30 | 0.65 |
| 13:YA:551[A]:THR:HG22 | 13:YC:558[A]:SER:HB3 | 1.79 | 0.65 |
| 13:YA:551[B]:THR:HG22 | 13:YC:558[B]:SER:HB3 | 1.78 | 0.65 |
| 14:YD:245[A]:ARG:NE | 14:YD:246[A]:ASP:OD1 | 2.25 | 0.65 |
| 13:YA:24[A]:LEU:HD23 | 14:YD:259[A]:LEU:HD22 | 1.78 | 0.65 |
| 14:YE:19[D]:SER:H | 14:YE:22[D]:ALA:HB3 | 1.60 | 0.65 |
| 14:YE:245[E]:ARG:NE | 14:YE:246[E]:ASP:OD1 | 2.25 | 0.65 |
| 13:YC:47[A]:ILE:HG23 | 14:YF:123[A]:PRO:HG3 | 1.77 | 0.65 |
| 14:YF:245[C]:ARG:NE | 14:YF:246[C]:ASP:OD1 | 2.25 | 0.65 |
| 1:A:522:LYS:HA | 1:A:534:VAL:HG23 | 1.78 | 0.65 |
| 5:AD:594:THR:OG1 | 5:AE:517:GLY:N | 2.28 | 0.65 |
| 5:AE:130:PHE:HB3 | 5:AE:151:ILE:HG22 | 1.76 | 0.65 |
| 7:AJ:330:ARG:NH2 | 7:AJ:336:GLU:OE2 | 2.22 | 0.65 |
| 7:AJ:509:GLY:HA3 | 7:BA:441:GLN:HE21 | 1.60 | 0.65 |
| 12:BG:233:ASP:OD1 | 12:BG:234:ASN:N | 2.29 | 0.65 |
| 1:BH:99:LEU:HG | 1:BH:211:ARG:HH12 | 1.59 | 0.65 |
| 1:BI:87:SER:OG | 1:BI:230:ILE:O | 2.11 | 0.65 |
| 2:BJ:539:LEU:HB3 | 2:BJ:541:TYR:H | 1.60 | 0.65 |
| 2:BJ:562:ASP:OD1 | 2:BJ:563:ASP:N | 2.30 | 0.65 |
| 2:BJ:940:GLY:O | 5:CF:21:LYS:NZ | 2.30 | 0.65 |
| 7:DB:498:SER:O | 7:DD:422:LYS:NZ | 2.29 | 0.65 |
| 11:DI:129:ASN:HB2 | 11:DI:132:VAL:HG12 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:92:ARG:HB3 | 3:ED:208:ILE:HG23 | 1.77 | 0.65 |
| 3:EE:51:GLU:OE2 | 3:EE:270:ARG:NH2 | 2.29 | 0.65 |
| 4:F:103:LEU:O | 4:H:69:LYS:NZ | 2.22 | 0.65 |
| 5:EJ:318:GLN:NE2 | 6:FB:4:LEU:O | 2.29 | 0.65 |
| 7:FE:220:SER:OG | 7:FG:228:ILE:O | 2.06 | 0.65 |
| 2:GF:981:GLN:OE1 | 2:GF:981:GLN:N | 2.29 | 0.65 |
| 5:HB:34:TYR:O | 5:HB:38:GLY:N | 2.26 | 0.65 |
| 7:HH:2:SER:O | 7:HH:6:TYR:N | 2.25 | 0.65 |
| 7:HI:81:LEU:O | 7:HI:85:LEU:N | 2.30 | 0.65 |
| 5:J:237:ASN:OD1 | 5:J:238:ILE:N | 2.29 | 0.65 |
| 5:K:221:GLU:OE2 | 5:K:233:ARG:NH2 | 2.29 | 0.65 |
| 5:K:270:LEU:HG | 6:N:108:LEU:HD21 | 1.79 | 0.65 |
| 7:O:472:ARG:NH2 | 5:FA:361:ASP:HB3 | 2.11 | 0.65 |
| 7:O:481:SER:OG | 7:P:449:GLY:O | 2.12 | 0.65 |
| 7:Q:325:TYR:HD1 | 7:Q:330:ARG:HA | 1.61 | 0.65 |
| 1:X:236:PHE:CE2 | 1:X:270:ILE:HD11 | 2.30 | 0.65 |
| 1:X:506:LYS:O | 1:X:509:SER:OG | 2.11 | 0.65 |
| 1:Y:77:GLU:OE2 | 1:Y:85:LEU:HB3 | 1.96 | 0.65 |
| 13:YA:24[D]:LEU:HD23 | 14:YD:259[D]:LEU:HD22 | 1.79 | 0.65 |
| 13:YA:24[E]:LEU:HD23 | 14:YD:259[E]:LEU:HD22 | 1.79 | 0.65 |
| 13:YC:38[A]:GLN:N | 13:YC:38[A]:GLN:OE1 | 2.30 | 0.65 |
| 13:YA:533[D]:ASN:HD22 | 13:YC:540[D]:GLY:HA3 | 1.62 | 0.65 |
| 14:YD:211[D]:MET:HE1 | 14:YD:231[D]:ALA:HB2 | 1.76 | 0.65 |
| 14:YE:215[A]:GLU:OE1 | 14:YF:100[A]:LYS:NZ | 2.29 | 0.65 |
| 11:V:178:ASN:N | 14:YF:217[C]:SER:O | 2.27 | 0.65 |
| 2:Z:134:TYR:OH | 2:Z:593:GLU:HG2 | 1.97 | 0.65 |
| 5:AE:491:ASN:HD22 | 5:AE:496:ASP:HB2 | 1.61 | 0.65 |
| 7:AJ:386:ASN:OD1 | 7:AJ:389:ASN:N | 2.29 | 0.65 |
| 7:AI:481:SER:OG | 7:AJ:449:GLY:O | 2.13 | 0.65 |
| 7:AJ:513:ARG:N | 7:BA:441:GLN:O | 2.20 | 0.65 |
| 1:BH:510:MET:HB3 | 1:BH:542:SER:HB3 | 1.79 | 0.65 |
| 2:BJ:344:THR:OG1 | 2:BJ:347:GLU:OE1 | 2.09 | 0.65 |
| 2:C:884:HIS:ND1 | 2:C:885:PRO:O | 2.30 | 0.65 |
| 3:CA:54:VAL:HG23 | 3:CB:5:SER:HA | 1.77 | 0.65 |
| 5:CG:237:ASN:OD1 | 5:CG:238:ILE:N | 2.29 | 0.65 |
| 5:CH:85:THR:HB | 5:CH:137:TYR:CE2 | 2.31 | 0.65 |
| 3:E:51:GLU:OE2 | 3:E:270:ARG:NH2 | 2.29 | 0.65 |
| 1:EB:521:ARG:O | 1:EB:533:ASP:HB2 | 1.97 | 0.65 |
| 3:ED:93:ARG:HH22 | 3:ED:110:ASP:HB3 | 1.62 | 0.65 |
| 5:EJ:237:ASN:OD1 | 5:EJ:238:ILE:N | 2.29 | 0.65 |
| 5:EJ:329:PHE:HB3 | 5:EJ:332:VAL:HB | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FB:60:HIS:NE2 | 6:FD:28:ASP:OD2 | 2.30 | 0.65 |
| 7:FE:176:ILE:HG12 | 7:FE:177:ALA:H | 1.61 | 0.65 |
| 7:FF:146:SER:H | 7:FF:149:GLN:HB2 | 1.61 | 0.65 |
| 7:FF:233:GLN:HE21 | 7:FF:237:ASN:HD21 | 1.44 | 0.65 |
| 7:FG:334:GLN:HG3 | 7:FG:337:ILE:HD12 | 1.78 | 0.65 |
| 1:GD:236:PHE:CE2 | 1:GD:270:ILE:HD11 | 2.30 | 0.65 |
| 1:GD:506:LYS:O | 1:GD:509:SER:OG | 2.11 | 0.65 |
| 2:GF:562:ASP:OD1 | 2:GF:563:ASP:N | 2.30 | 0.65 |
| 5:HB:164:ARG:HG3 | 5:HB:245:GLU:HG2 | 1.78 | 0.65 |
| 5:HB:193:VAL:HG13 | 5:HB:199:GLU:HB3 | 1.78 | 0.65 |
| 5:HC:137:TYR:HA | 5:HC:143:TRP:CD1 | 2.32 | 0.65 |
| 5:HD:85:THR:HB | 5:HD:137:TYR:CE2 | 2.31 | 0.65 |
| 5:HD:177:PHE:HD2 | 5:HD:230:ILE:HD11 | 1.61 | 0.65 |
| 5:HD:221:GLU:OE2 | 5:HD:233:ARG:NH2 | 2.29 | 0.65 |
| 6:HE:39:THR:OG1 | 6:HE:42:GLN:OE1 | 2.14 | 0.65 |
| 6:HF:16:ASP:OD2 | 6:HF:45:LYS:NZ | 2.29 | 0.65 |
| 6:HF:39:THR:OG1 | 6:HF:42:GLN:OE1 | 2.14 | 0.65 |
| 7:HH:447:HIS:HD2 | 7:HI:447:HIS:CD2 | 2.13 | 0.65 |
| 11:IE:129:ASN:HB2 | 11:IE:132:VAL:HG12 | 1.77 | 0.65 |
| 9:T:59:ASP:HA | 9:T:62:PHE:HB3 | 1.77 | 0.65 |
| 10:U:214:ARG:NH1 | 12:W:246:ARG:HH12 | 1.94 | 0.65 |
| 13:YC:38[F]:GLN:N | 13:YC:38[F]:GLN:OE1 | 2.29 | 0.65 |
| 13:YB:95[F]:ILE:HD11 | 13:YC:83[F]:TYR:CZ | 2.31 | 0.65 |
| 2:Z:770:ILE:HG22 | 2:Z:842:VAL:H | 1.58 | 0.65 |
| 5:AE:318:GLN:HE22 | 6:AG:8:ALA:N | 1.95 | 0.65 |
| 5:AE:340:VAL:HG23 | 5:AE:341:GLU:HG3 | 1.79 | 0.65 |
| 7:AJ:130:GLU:HG2 | 7:BA:139:ASN:HD21 | 1.61 | 0.65 |
| 7:AI:143:LYS:HA | 7:AJ:134:SER:HB2 | 1.79 | 0.65 |
| 7:BA:375:TYR:OH | 7:BA:391:GLY:O | 2.14 | 0.65 |
| 1:BI:77:GLU:OE2 | 1:BI:85:LEU:HB3 | 1.96 | 0.65 |
| 2:BJ:897:THR:HG22 | 3:CB:329:ASN:HB2 | 1.78 | 0.65 |
| 2:C:562:ASP:OD1 | 2:C:563:ASP:N | 2.30 | 0.65 |
| 5:CG:71:ASN:OD1 | 5:CG:73:SER:N | 2.23 | 0.65 |
| 7:DB:41:PRO:O | 7:DB:45:ASN:ND2 | 2.29 | 0.65 |
| 12:DJ:15:ASP:CG | 12:DJ:16:PHE:H | 2.00 | 0.65 |
| 3:E:170:PRO:HB3 | 3:E:188:TRP:CD1 | 2.30 | 0.65 |
| 4:EG:106:CYS:SG | 4:EG:149:ARG:NH2 | 2.67 | 0.65 |
| 5:EJ:111:ALA:HB2 | 5:EJ:117:ILE:HG23 | 1.78 | 0.65 |
| 5:FA:340:VAL:HG23 | 5:FA:341:GLU:HG3 | 1.79 | 0.65 |
| 5:FA:318:GLN:HE22 | 6:FC:8:ALA:N | 1.94 | 0.65 |
| 7:FE:41:PRO:O | 7:FE:45:ASN:ND2 | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FF:486:ASP:HB2 | 7:FG:444:TYR:HB2 | 1.77 | 0.65 |
| 9:FJ:10:ASP:OD1 | 9:FJ:11:ILE:N | 2.28 | 0.65 |
| 2:GF:752:TYR:OH | 2:GF:878:ASP:OD2 | 2.11 | 0.65 |
| 3:GG:93:ARG:HH22 | 3:GG:110:ASP:HB3 | 1.62 | 0.65 |
| 7:HH:193:LEU:HD13 | 7:HI:206:GLU:HG3 | 1.79 | 0.65 |
| 7:HI:132:ARG:NH2 | 7:HI:139:ASN:OD1 | 2.30 | 0.65 |
| 5:J:117:ILE:HG22 | 5:J:143:TRP:HE3 | 1.62 | 0.65 |
| 7:O:2:SER:O | 7:O:6:TYR:N | 2.25 | 0.65 |
| 5:K:196:ARG:NH1 | 7:P:8:HIS:HB3 | 2.12 | 0.65 |
| 1:X:156:ASP:OD1 | 1:X:157:LYS:N | 2.29 | 0.65 |
| 13:YA:38[E]:GLN:OE1 | 13:YA:38[E]:GLN:N | 2.30 | 0.65 |
| 14:YD:19[F]:SER:H | 14:YD:22[F]:ALA:HB3 | 1.60 | 0.65 |
| 14:YF:19[B]:SER:H | 14:YF:22[B]:ALA:HB3 | 1.60 | 0.65 |
| 14:YF:245[F]:ARG:NE | 14:YF:246[F]:ASP:OD1 | 2.25 | 0.65 |
| 14:YF:288[F]:TYR:OH | 14:YF:371[F]:LYS:NZ | 2.27 | 0.65 |
| 1:A:145:PHE:HB2 | 1:A:168:ALA:O | 1.97 | 0.65 |
| 5:AE:344:VAL:HG12 | 5:AE:349:TRP:HB3 | 1.77 | 0.65 |
| 1:BH:145:PHE:HB2 | 1:BH:168:ALA:O | 1.97 | 0.65 |
| 1:BI:543:THR:HG21 | 1:BI:551:GLY:HA3 | 1.78 | 0.65 |
| 2:BJ:712:ASN:OD1 | 2:BJ:720:ARG:NH1 | 2.30 | 0.65 |
| 5:CH:340:VAL:HG23 | 5:CH:341:GLU:HG3 | 1.79 | 0.65 |
| 3:D:93:ARG:HH22 | 3:D:110:ASP:HB3 | 1.62 | 0.65 |
| 6:CI:60:HIS:NE2 | 6:DA:28:ASP:OD2 | 2.30 | 0.65 |
| 7:DB:289:GLN:HA | 7:DC:287:VAL:HA | 1.77 | 0.65 |
| 7:DC:497:ASN:H | 7:DC:500:TYR:HB2 | 1.61 | 0.65 |
| 1:EA:145:PHE:HB2 | 1:EA:168:ALA:O | 1.97 | 0.65 |
| 2:EC:950:GLU:OE1 | 2:EC:950:GLU:N | 2.24 | 0.65 |
| 2:EC:87:GLN:NE2 | 3:ED:158:GLY:HA2 | 2.10 | 0.65 |
| 5:FA:221:GLU:OE2 | 5:FA:233:ARG:NH2 | 2.29 | 0.65 |
| 6:FD:39:THR:OG1 | 6:FD:42:GLN:OE1 | 2.14 | 0.65 |
| 7:FE:143:LYS:HA | 7:FF:134:SER:HB2 | 1.79 | 0.65 |
| 7:FE:351:ALA:O | 7:FE:520:ASN:ND2 | 2.29 | 0.65 |
| 9:FJ:98:VAL:N | 9:FJ:103:THR:O | 2.26 | 0.65 |
| 4:HA:106:CYS:SG | 4:HA:149:ARG:NH2 | 2.67 | 0.65 |
| 5:HC:170:GLU:HA | 5:HC:238:ILE:HG13 | 1.76 | 0.65 |
| 5:HC:237:ASN:OD1 | 5:HC:238:ILE:N | 2.29 | 0.65 |
| 7:HI:386:ASN:OD1 | 7:HI:389:ASN:N | 2.29 | 0.65 |
| 7:HI:509:GLY:HA3 | 7:HJ:441:GLN:HE21 | 1.61 | 0.65 |
| 6:L:11:ILE:HA | 6:N:7:LYS:HD3 | 1.79 | 0.65 |
| 7:O:297:TYR:N | 7:Q:290:GLN:O | 2.25 | 0.65 |
| 13:YA:24[F]:LEU:HD23 | 14:YD:259[F]:LEU:HD22 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:403[B]:PHE:HB3 | 13:YC:399[B]:HIS:CD2 | 2.30 | 0.65 |
| 13:YB:442[B]:THR:HG21 | 13:YC:438[B]:LEU:HD22 | 1.79 | 0.65 |
| 14:YD:211[A]:MET:HE1 | 14:YD:231[A]:ALA:HB2 | 1.78 | 0.65 |
| 14:YD:366[D]:THR:O | 14:YD:369[D]:PRO:HD3 | 1.96 | 0.65 |
| 14:YD:366[E]:THR:O | 14:YD:369[E]:PRO:HD3 | 1.96 | 0.65 |
| 14:YE:288[B]:TYR:OH | 14:YE:371[B]:LYS:NZ | 2.27 | 0.65 |
| 14:YF:366[E]:THR:O | 14:YF:369[E]:PRO:HD3 | 1.96 | 0.65 |
| 14:YF:366[F]:THR:O | 14:YF:369[F]:PRO:HD3 | 1.96 | 0.65 |
| 2:Z:990:MET:HG3 | 2:Z:992:PRO:HD3 | 1.78 | 0.65 |
| 1:A:156:ASP:OD1 | 1:A:157:LYS:N | 2.29 | 0.65 |
| 1:A:18:PRO:HG3 | 2:C:701:TRP:CD1 | 2.32 | 0.65 |
| 5:AC:263:ILE:HG22 | 5:AC:381:ILE:HB | 1.79 | 0.65 |
| 7:BA:67:ILE:HA | 7:BA:84:ARG:HH21 | 1.62 | 0.65 |
| 2:C:52:ASN:OD1 | 2:C:53:GLN:N | 2.27 | 0.65 |
| 5:CG:312:ARG:HG2 | 5:CG:317:LEU:HA | 1.78 | 0.65 |
| 5:CH:491:ASN:HD22 | 5:CH:496:ASP:HB2 | 1.61 | 0.65 |
| 3:E:292:ALA:HB1 | 3:E:297:TYR:HE2 | 1.62 | 0.65 |
| 1:EA:156:ASP:OD1 | 1:EA:157:LYS:N | 2.29 | 0.65 |
| 5:EJ:189:ASN:HD21 | 5:FA:150:GLN:NE2 | 1.95 | 0.65 |
| 5:EJ:175:THR:O | 5:EJ:232:LEU:N | 2.30 | 0.65 |
| 5:FA:316:ILE:HG22 | 5:FA:318:GLN:HG3 | 1.78 | 0.65 |
| 5:FA:9:ASN:OD1 | 5:FA:10:VAL:N | 2.30 | 0.65 |
| 1:GD:396:LEU:O | 1:GD:399:TYR:N | 2.30 | 0.65 |
| 1:GD:7:ASN:HD22 | 2:GF:634:PRO:HG2 | 1.61 | 0.65 |
| 5:HC:329:PHE:HB3 | 5:HC:332:VAL:HB | 1.79 | 0.65 |
| 7:HI:149:GLN:O | 7:HI:153:GLY:HA2 | 1.95 | 0.65 |
| 7:HI:233:GLN:HE21 | 7:HI:237:ASN:HD21 | 1.44 | 0.65 |
| 7:HJ:177:ALA:HB3 | 7:HJ:178:PRO:HD3 | 1.78 | 0.65 |
| 5:K:491:ASN:HD22 | 5:K:496:ASP:HB2 | 1.61 | 0.65 |
| 7:P:132:ARG:NH2 | 7:P:139:ASN:OD1 | 2.30 | 0.65 |
| 12:W:15:ASP:CG | 12:W:16:PHE:H | 2.00 | 0.65 |
| 1:Y:543:THR:OG1 | 1:Y:544:ASP:N | 2.29 | 0.65 |
| 13:YA:47[B]:ILE:HG23 | 14:YD:123[B]:PRO:HG3 | 1.78 | 0.65 |
| 13:YB:38[D]:GLN:OE1 | 13:YB:38[D]:GLN:N | 2.29 | 0.65 |
| 13:YB:95[B]:ILE:HD11 | 13:YC:83[B]:TYR:CZ | 2.32 | 0.65 |
| 14:YD:312[C]:THR:OG1 | 14:YD:313[C]:ILE:N | 2.29 | 0.65 |
| 13:YC:47[C]:ILE:HG23 | 14:YF:123[C]:PRO:HG3 | 1.79 | 0.65 |
| 2:Z:436:THR:HG22 | 2:Z:441:VAL:HG12 | 1.79 | 0.65 |
| 1:A:578:ASN:OD1 | 1:A:579:LYS:N | 2.30 | 0.65 |
| 4:AB:106:CYS:SG | 4:AB:149:ARG:NH2 | 2.67 | 0.65 |
| 7:AI:86:SER:HA | 7:AI:97:LEU:HD12 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:132:ARG:NH2 | 7:AJ:139:ASN:OD1 | 2.30 | 0.65 |
| 7:AJ:497:ASN:H | 7:AJ:500:TYR:HB2 | 1.60 | 0.65 |
| 1:B:411:PRO:HG2 | 1:B:413:TYR:CE1 | 2.32 | 0.65 |
| 1:BI:411:PRO:HG2 | 1:BI:413:TYR:CE1 | 2.32 | 0.65 |
| 2:BJ:389:ASN:HB3 | 2:BJ:392:THR:HG22 | 1.77 | 0.65 |
| 2:C:232:PRO:HG3 | 2:C:237:VAL:HG22 | 1.79 | 0.65 |
| 2:C:712:ASN:OD1 | 2:C:720:ARG:NH1 | 2.30 | 0.65 |
| 4:CD:106:CYS:SG | 4:CD:149:ARG:NH2 | 2.67 | 0.65 |
| 5:CG:137:TYR:HA | 5:CG:143:TRP:CD1 | 2.32 | 0.65 |
| 5:CG:89:TYR:O | 5:CG:91:LYS:N | 2.30 | 0.65 |
| 6:CI:39:THR:OG1 | 6:CI:42:GLN:OE1 | 2.14 | 0.65 |
| 5:CH:318:GLN:HE22 | 6:CJ:8:ALA:N | 1.95 | 0.65 |
| 7:DB:347:MET:HE3 | 7:DC:347:MET:HB3 | 1.77 | 0.65 |
| 7:DB:449:GLY:HA2 | 7:DC:484:THR:HG22 | 1.79 | 0.65 |
| 7:DC:81:LEU:O | 7:DC:85:LEU:N | 2.30 | 0.65 |
| 7:DD:67:ILE:HA | 7:DD:84:ARG:HH21 | 1.62 | 0.65 |
| 12:DJ:233:ASP:OD1 | 12:DJ:234:ASN:N | 2.29 | 0.65 |
| 2:EC:232:PRO:HG3 | 2:EC:237:VAL:HG22 | 1.79 | 0.65 |
| 2:EC:562:ASP:OD1 | 2:EC:563:ASP:N | 2.30 | 0.65 |
| 6:FB:39:THR:OG1 | 6:FB:42:GLN:OE1 | 2.14 | 0.65 |
| 6:FC:39:THR:OG1 | 6:FC:42:GLN:OE1 | 2.14 | 0.65 |
| 7:FF:149:GLN:O | 7:FF:153:GLY:HA2 | 1.95 | 0.65 |
| 7:FG:497:ASN:H | 7:FG:500:TYR:HB2 | 1.62 | 0.65 |
| 7:HH:496:ARG:NH1 | 7:HH:501:THR:OG1 | 2.29 | 0.65 |
| 7:HH:86:SER:HA | 7:HH:97:LEU:HD12 | 1.79 | 0.65 |
| 7:HJ:497:ASN:H | 7:HJ:500:TYR:HB2 | 1.62 | 0.65 |
| 5:K:555:CYS:O | 5:K:556:GLN:HG2 | 1.97 | 0.65 |
| 1:Y:230:ILE:HD13 | 2:Z:691:ARG:HG3 | 1.78 | 0.65 |
| 13:YA:38[F]:GLN:OE1 | 13:YA:38[F]:GLN:N | 2.29 | 0.65 |
| 13:YB:38[F]:GLN:OE1 | 13:YB:38[F]:GLN:N | 2.29 | 0.65 |
| 13:YC:38[D]:GLN:N | 13:YC:38[D]:GLN:OE1 | 2.29 | 0.65 |
| 14:YD:288[D]:TYR:OH | 14:YD:371[D]:LYS:NZ | 2.27 | 0.65 |
| 14:YD:366[C]:THR:O | 14:YD:369[C]:PRO:HD3 | 1.96 | 0.65 |
| 11:IE:178:ASN:N | 14:YE:217[D]:SER:O | 2.28 | 0.65 |
| 14:YE:366[A]:THR:O | 14:YE:369[A]:PRO:HD3 | 1.96 | 0.65 |
| 2:Z:909:THR:OG1 | 2:Z:910:GLU:OE1 | 2.11 | 0.65 |
| 4:AA:106:CYS:SG | 4:AA:149:ARG:NH2 | 2.67 | 0.65 |
| 5:AD:89:TYR:O | 5:AD:91:LYS:N | 2.30 | 0.65 |
| 5:AC:241:THR:HG21 | 5:AE:200:LEU:HD13 | 1.79 | 0.65 |
| 5:AD:326:MET:HE3 | 5:AE:279:SER:HA | 1.79 | 0.65 |
| 5:AE:9:ASN:OD1 | 5:AE:10:VAL:N | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:361:GLN:HG2 | 1:B:455:PHE:CE2 | 2.31 | 0.65 |
| 7:BA:497:ASN:H | 7:BA:500:TYR:HB2 | 1.62 | 0.65 |
| 7:AI:441:GLN:NE2 | 7:BA:509:GLY:HA3 | 2.12 | 0.65 |
| 9:BD:85:GLU:OE2 | 9:BD:87:ARG:NE | 2.29 | 0.65 |
| 2:C:1014:ASP:HA | 2:C:1027:GLN:HB3 | 1.79 | 0.65 |
| 2:C:67:PHE:HE2 | 2:C:69:PHE:HB2 | 1.60 | 0.65 |
| 2:C:68:PHE:CZ | 2:C:564:GLY:HA2 | 2.32 | 0.65 |
| 2:C:872:SER:N | 2:C:894:THR:HG21 | 2.11 | 0.65 |
| 3:CA:93:ARG:HH22 | 3:CA:110:ASP:HB3 | 1.62 | 0.65 |
| 5:CF:312:ARG:HB2 | 5:CF:382:ASN:HB2 | 1.78 | 0.65 |
| 5:CH:270:LEU:HG | 6:DA:108:LEU:HD21 | 1.79 | 0.65 |
| 5:CH:316:ILE:HG22 | 5:CH:318:GLN:HG3 | 1.78 | 0.65 |
| 7:DC:233:GLN:HE21 | 7:DC:237:ASN:HD21 | 1.44 | 0.65 |
| 7:DD:325:TYR:HD1 | 7:DD:330:ARG:HA | 1.61 | 0.65 |
| 7:DC:509:GLY:HA3 | 7:DD:441:GLN:HE21 | 1.60 | 0.65 |
| 5:CF:234:GLN:HE22 | 7:DD:9:VAL:HG21 | 1.61 | 0.65 |
| 1:EA:522:LYS:HA | 1:EA:534:VAL:HG23 | 1.78 | 0.65 |
| 1:EB:77:GLU:OE2 | 1:EB:85:LEU:HB3 | 1.96 | 0.65 |
| 2:EC:374:LYS:NZ | 2:EC:499:GLU:OE2 | 2.18 | 0.65 |
| 2:EC:712:ASN:OD1 | 2:EC:720:ARG:NH1 | 2.30 | 0.65 |
| 7:FE:101:SER:HB3 | 7:FE:120:LYS:HE3 | 1.79 | 0.65 |
| 7:FF:132:ARG:NH2 | 7:FF:139:ASN:OD1 | 2.30 | 0.65 |
| 12:GC:233:ASP:OD1 | 12:GC:234:ASN:N | 2.29 | 0.65 |
| 2:GF:117:GLN:O | 2:GF:596:SER:OG | 2.15 | 0.65 |
| 5:HC:175:THR:O | 5:HC:232:LEU:N | 2.30 | 0.65 |
| 7:Q:497:ASN:H | 7:Q:500:TYR:HB2 | 1.62 | 0.65 |
| 13:YA:30[A]:ARG:HB2 | 13:YA:52[A]:LEU:HD21 | 1.79 | 0.65 |
| 13:YB:30[E]:ARG:HB2 | 13:YB:52[E]:LEU:HD21 | 1.79 | 0.65 |
| 13:YB:95[D]:ILE:HD11 | 13:YC:83[D]:TYR:CZ | 2.32 | 0.65 |
| 13:YC:30[C]:ARG:HB2 | 13:YC:52[C]:LEU:HD21 | 1.79 | 0.65 |
| 13:YA:514[D]:VAL:O | 13:YC:522[D]:VAL:HA | 1.96 | 0.65 |
| 13:YA:550[F]:TRP:CD1 | 13:YC:554[F]:MET:HE2 | 2.32 | 0.65 |
| 13:YA:47[F]:ILE:HG23 | 14:YD:123[F]:PRO:HG3 | 1.79 | 0.65 |
| 14:YD:366[F]:THR:O | 14:YD:369[F]:PRO:HD3 | 1.96 | 0.65 |
| 14:YE:312[D]:THR:OG1 | 14:YE:313[D]:ILE:N | 2.29 | 0.65 |
| 14:YE:366[D]:THR:O | 14:YE:369[D]:PRO:HD3 | 1.96 | 0.65 |
| 14:YF:312[B]:THR:OG1 | 14:YF:313[B]:ILE:N | 2.29 | 0.65 |
| 14:YF:366[B]:THR:O | 14:YF:369[B]:PRO:HD3 | 1.96 | 0.65 |
| 2:Z:81:ARG:HD2 | 2:Z:94:TRP:HB3 | 1.77 | 0.65 |
| 1:B:77:GLU:OE2 | 1:B:85:LEU:HB3 | 1.96 | 0.65 |
| 12:BG:119:ASN:O | 12:BG:122:GLY:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:34:ILE:HG23 | 1:BH:48:PHE:HD2 | 1.62 | 0.65 |
| 1:BH:578:ASN:OD1 | 1:BH:579:LYS:N | 2.30 | 0.65 |
| 1:BI:543:THR:OG1 | 1:BI:544:ASP:N | 2.29 | 0.65 |
| 2:BJ:232:PRO:HG3 | 2:BJ:237:VAL:HG22 | 1.79 | 0.65 |
| 5:CG:111:ALA:HB2 | 5:CG:117:ILE:HG23 | 1.78 | 0.65 |
| 5:CF:241:THR:HG21 | 5:CH:200:LEU:HD13 | 1.79 | 0.65 |
| 3:D:92:ARG:HB3 | 3:D:208:ILE:HG23 | 1.77 | 0.65 |
| 6:DA:39:THR:OG1 | 6:DA:42:GLN:OE1 | 2.14 | 0.65 |
| 7:DB:101:SER:HB3 | 7:DB:120:LYS:HE3 | 1.79 | 0.65 |
| 8:BB:56:ARG:HD3 | 8:DE:64:ARG:HD3 | 1.78 | 0.65 |
| 3:D:54:VAL:HG23 | 3:E:5:SER:HA | 1.77 | 0.65 |
| 1:BI:38:ASN:ND2 | 1:EA:264:GLN:OE1 | 2.30 | 0.65 |
| 1:EA:236:PHE:CE2 | 1:EA:270:ILE:HD11 | 2.30 | 0.65 |
| 1:EA:337:GLN:HG3 | 1:EB:334:GLU:HG2 | 1.79 | 0.65 |
| 1:EA:510:MET:HB3 | 1:EA:542:SER:HB3 | 1.79 | 0.65 |
| 2:EC:436:THR:HG22 | 2:EC:441:VAL:HG12 | 1.78 | 0.65 |
| 5:EI:193:VAL:HG13 | 5:EI:199:GLU:HB3 | 1.78 | 0.65 |
| 5:EI:263:ILE:HG22 | 5:EI:381:ILE:HB | 1.79 | 0.65 |
| 5:EI:264:ARG:HB3 | 5:FA:326:MET:CE | 2.28 | 0.65 |
| 2:GF:712:ASN:OD1 | 2:GF:720:ARG:NH1 | 2.30 | 0.65 |
| 5:HC:119:GLY:H | 5:HC:142:ARG:HH22 | 1.44 | 0.65 |
| 5:HC:223:VAL:HB | 5:HC:224:PRO:HD3 | 1.78 | 0.65 |
| 9:IC:89:ASP:HB2 | 9:IC:113:ILE:HD13 | 1.80 | 0.65 |
| 7:O:330:ARG:NH2 | 7:O:336:GLU:OE2 | 2.27 | 0.65 |
| 7:O:86:SER:HA | 7:O:97:LEU:HD12 | 1.79 | 0.65 |
| 1:X:543:THR:HG21 | 1:X:552:LYS:H | 1.62 | 0.65 |
| 13:YA:30[B]:ARG:HB2 | 13:YA:52[B]:LEU:HD21 | 1.79 | 0.65 |
| 13:YA:533[E]:ASN:HD22 | 13:YC:540[E]:GLY:HA3 | 1.61 | 0.65 |
| 13:YB:30[B]:ARG:HB2 | 13:YB:52[B]:LEU:HD21 | 1.79 | 0.65 |
| 13:YB:442[C]:THR:HG21 | 13:YC:438[C]:LEU:HD22 | 1.79 | 0.65 |
| 13:YB:538[E]:VAL:HG11 | 13:YC:534[E]:LEU:HB2 | 1.79 | 0.65 |
| 13:YC:24[C]:LEU:HD23 | 14:YF:259[C]:LEU:HD22 | 1.79 | 0.65 |
| 13:YB:442[F]:THR:HG21 | 13:YC:438[F]:LEU:HD22 | 1.79 | 0.65 |
| 13:YB:538[B]:VAL:HG11 | 13:YC:534[B]:LEU:HB2 | 1.79 | 0.65 |
| 13:YA:551[E]:THR:HG22 | 13:YC:558[E]:SER:HB3 | 1.78 | 0.65 |
| 14:YE:19[A]:SER:H | 14:YE:22[A]:ALA:HB3 | 1.60 | 0.65 |
| 14:YF:19[E]:SER:H | 14:YF:22[E]:ALA:HB3 | 1.60 | 0.65 |
| 2:Z:562:ASP:OD1 | 2:Z:563:ASP:N | 2.30 | 0.65 |
| 2:Z:68:PHE:CZ | 2:Z:564:GLY:HA2 | 2.32 | 0.65 |
| 5:AD:137:TYR:HA | 5:AD:143:TRP:CD1 | 2.32 | 0.64 |
| 7:AI:193:LEU:HD13 | 7:AJ:206:GLU:HG3 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:257:ILE:HG12 | 1:BI:331:ILE:HD11 | 1.79 | 0.64 |
| 2:BJ:52:ASN:OD1 | 2:BJ:53:GLN:N | 2.27 | 0.64 |
| 3:CB:42:GLY:HA2 | 3:CB:76:MET:HG2 | 1.79 | 0.64 |
| 4:CC:106:CYS:SG | 4:CC:149:ARG:NH2 | 2.67 | 0.64 |
| 10:DH:214:ARG:NH1 | 12:DJ:246:ARG:HH12 | 1.94 | 0.64 |
| 2:EC:81:ARG:HD2 | 2:EC:94:TRP:HB3 | 1.78 | 0.64 |
| 5:EJ:223:VAL:HB | 5:EJ:224:PRO:HD3 | 1.78 | 0.64 |
| 5:EJ:147:LYS:HB2 | 5:FA:153:LYS:HB2 | 1.79 | 0.64 |
| 9:FJ:85:GLU:OE2 | 9:FJ:87:ARG:NE | 2.29 | 0.64 |
| 1:GD:553:VAL:N | 1:GD:593:GLY:O | 2.21 | 0.64 |
| 1:GD:8:TYR:OH | 1:GD:19:GLU:HG3 | 1.98 | 0.64 |
| 1:GE:411:PRO:HG2 | 1:GE:413:TYR:CE1 | 2.32 | 0.64 |
| 1:GE:77:GLU:OE2 | 1:GE:85:LEU:HB3 | 1.96 | 0.64 |
| 7:HH:212:PRO:HB3 | 7:HI:199:VAL:HA | 1.78 | 0.64 |
| 5:K:186:TYR:OH | 5:K:190:ASN:O | 2.12 | 0.64 |
| 5:K:361:ASP:HB3 | 7:AI:472:ARG:NH2 | 2.12 | 0.64 |
| 7:Q:67:ILE:HA | 7:Q:84:ARG:HH21 | 1.62 | 0.64 |
| 9:T:89:ASP:HB2 | 9:T:113:ILE:HD13 | 1.80 | 0.64 |
| 1:Y:521:ARG:O | 1:Y:533:ASP:HB2 | 1.97 | 0.64 |
| 13:YB:232[D]:ASN:CB | 13:YC:407[D]:PRO:HB3 | 2.27 | 0.64 |
| 13:YB:418[E]:THR:HG21 | 13:YC:428[E]:GLY:HA3 | 1.79 | 0.64 |
| 13:YB:442[A]:THR:HG21 | 13:YC:438[A]:LEU:HD22 | 1.79 | 0.64 |
| 13:YA:533[C]:ASN:HD22 | 13:YC:540[C]:GLY:HA3 | 1.61 | 0.64 |
| 13:YC:47[D]:ILE:HG23 | 14:YF:123[D]:PRO:HG3 | 1.79 | 0.64 |
| 14:YF:366[A]:THR:O | 14:YF:369[A]:PRO:HD3 | 1.96 | 0.64 |
| 2:Z:232:PRO:HG3 | 2:Z:237:VAL:HG22 | 1.79 | 0.64 |
| 1:X:341:THR:HG21 | 2:Z:881:ARG:O | 1.98 | 0.64 |
| 2:Z:872:SER:N | 2:Z:894:THR:HG21 | 2.11 | 0.64 |
| 1:A:396:LEU:O | 1:A:399:TYR:N | 2.30 | 0.64 |
| 1:A:8:TYR:OH | 1:A:19:GLU:HG3 | 1.98 | 0.64 |
| 5:AC:397:ASP:O | 5:AC:401:ASP:N | 2.19 | 0.64 |
| 5:AD:111:ALA:HB2 | 5:AD:117:ILE:HG23 | 1.78 | 0.64 |
| 7:AI:176:ILE:HG12 | 7:AI:177:ALA:H | 1.62 | 0.64 |
| 7:AI:289:GLN:HA | 7:AJ:287:VAL:HA | 1.78 | 0.64 |
| 1:A:7:ASN:HD22 | 2:C:634:PRO:HG2 | 1.62 | 0.64 |
| 5:CG:223:VAL:HB | 5:CG:224:PRO:HD3 | 1.78 | 0.64 |
| 5:CG:175:THR:O | 5:CG:232:LEU:N | 2.30 | 0.64 |
| 5:CH:9:ASN:OD1 | 5:CH:10:VAL:N | 2.30 | 0.64 |
| 7:DC:150:ALA:HB3 | 7:DC:168:LEU:HD13 | 1.78 | 0.64 |
| 1:EA:396:LEU:O | 1:EA:399:TYR:N | 2.30 | 0.64 |
| 2:EC:186:ASP:OD1 | 2:EC:187:ILE:N | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:EE:42:GLY:HA2 | 3:EE:76:MET:HG2 | 1.79 | 0.64 |
| 5:EI:38:GLY:HA2 | 5:EI:43:PRO:HA | 1.80 | 0.64 |
| 1:GD:578:ASN:OD1 | 1:GD:579:LYS:N | 2.30 | 0.64 |
| 2:GF:134:TYR:OH | 2:GF:593:GLU:HG2 | 1.97 | 0.64 |
| 2:GF:872:SER:N | 2:GF:894:THR:HG21 | 2.11 | 0.64 |
| 2:GF:897:THR:HG22 | 3:GH:329:ASN:HB2 | 1.79 | 0.64 |
| 3:GH:170:PRO:HB3 | 3:GH:188:TRP:CD1 | 2.30 | 0.64 |
| 5:HB:263:ILE:HG22 | 5:HB:381:ILE:HB | 1.79 | 0.64 |
| 5:HD:555:CYS:O | 5:HD:556:GLN:HG2 | 1.97 | 0.64 |
| 7:HH:170:ILE:HD13 | 7:HI:172:LEU:HD22 | 1.78 | 0.64 |
| 7:HJ:67:ILE:HA | 7:HJ:84:ARG:HH21 | 1.62 | 0.64 |
| 5:J:175:THR:O | 5:J:232:LEU:N | 2.30 | 0.64 |
| 5:K:318:GLN:HE22 | 6:M:8:ALA:N | 1.95 | 0.64 |
| 7:O:418:ASP:OD1 | 7:O:422:LYS:N | 2.30 | 0.64 |
| 7:O:496:ARG:NH1 | 7:O:501:THR:OG1 | 2.29 | 0.64 |
| 7:O:143:LYS:HA | 7:P:134:SER:HB2 | 1.79 | 0.64 |
| 1:Y:361:GLN:HG2 | 1:Y:455:PHE:CE2 | 2.31 | 0.64 |
| 13:YB:30[F]:ARG:HB2 | 13:YB:52[F]:LEU:HD21 | 1.79 | 0.64 |
| 13:YB:95[C]:ILE:HD11 | 13:YC:83[C]:TYR:CZ | 2.32 | 0.64 |
| 14:YD:215[E]:GLU:OE1 | 14:YE:100[E]:LYS:NZ | 2.30 | 0.64 |
| 14:YE:312[B]:THR:OG1 | 14:YE:313[B]:ILE:N | 2.29 | 0.64 |
| 14:YE:366[B]:THR:O | 14:YE:369[B]:PRO:HD3 | 1.96 | 0.64 |
| 14:YE:366[C]:THR:O | 14:YE:369[C]:PRO:HD3 | 1.96 | 0.64 |
| 14:YF:312[E]:THR:OG1 | 14:YF:313[E]:ILE:N | 2.30 | 0.64 |
| 2:Z:712:ASN:OD1 | 2:Z:720:ARG:NH1 | 2.30 | 0.64 |
| 5:AD:186:TYR:HE1 | 5:AD:246:THR:HA | 1.63 | 0.64 |
| 5:AD:317:LEU:HD13 | 5:AE:312:ARG:HH22 | 1.62 | 0.64 |
| 5:AE:555:CYS:O | 5:AE:556:GLN:HG2 | 1.97 | 0.64 |
| 7:AI:101:SER:HB3 | 7:AI:120:LYS:HE3 | 1.79 | 0.64 |
| 7:AI:496:ARG:NH1 | 7:AI:501:THR:OG1 | 2.29 | 0.64 |
| 7:AJ:150:ALA:HB3 | 7:AJ:168:LEU:HD13 | 1.78 | 0.64 |
| 7:DB:441:GLN:NE2 | 7:DD:509:GLY:HA3 | 2.13 | 0.64 |
| 7:DC:132:ARG:NH2 | 7:DC:139:ASN:OD1 | 2.30 | 0.64 |
| 7:DB:207:GLY:HA2 | 7:DD:193:LEU:HD11 | 1.80 | 0.64 |
| 1:EA:525:ASN:O | 1:EA:528:THR:OG1 | 2.11 | 0.64 |
| 1:EB:543:THR:HG21 | 1:EB:551:GLY:HA3 | 1.78 | 0.64 |
| 2:EC:68:PHE:CZ | 2:EC:564:GLY:HA2 | 2.32 | 0.64 |
| 3:EE:292:ALA:HB1 | 3:EE:297:TYR:HE2 | 1.62 | 0.64 |
| 5:EJ:198:ASN:HD22 | 5:FA:194:LYS:HD3 | 1.61 | 0.64 |
| 5:FA:305:ASN:HB3 | 5:FA:388:ASN:HB2 | 1.79 | 0.64 |
| 7:FE:141:VAL:HG22 | 7:FF:139:ASN:HB2 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:2:SER:O | 7:FE:6:TYR:N | 2.25 | 0.64 |
| 1:GD:424:TYR:HE2 | 1:GD:655:LEU:HD13 | 1.63 | 0.64 |
| 2:GF:228:ARG:HH22 | 5:HD:559:PRO:HB3 | 1.61 | 0.64 |
| 5:HC:117:ILE:HG22 | 5:HC:143:TRP:HE3 | 1.62 | 0.64 |
| 5:HD:316:ILE:HG22 | 5:HD:318:GLN:HG3 | 1.77 | 0.64 |
| 5:K:305:ASN:HB3 | 5:K:388:ASN:HB2 | 1.79 | 0.64 |
| 13:YA:30[D]:ARG:HB2 | 13:YA:52[D]:LEU:HD21 | 1.79 | 0.64 |
| 13:YA:38[C]:GLN:N | 13:YA:38[C]:GLN:OE1 | 2.29 | 0.64 |
| 13:YB:38[B]:GLN:N | 13:YB:38[B]:GLN:OE1 | 2.30 | 0.64 |
| 13:YC:24[B]:LEU:HD23 | 14:YF:259[B]:LEU:HD22 | 1.79 | 0.64 |
| 13:YC:30[D]:ARG:HB2 | 13:YC:52[D]:LEU:HD21 | 1.79 | 0.64 |
| 13:YC:30[F]:ARG:HB2 | 13:YC:52[F]:LEU:HD21 | 1.79 | 0.64 |
| 14:YD:19[C]:SER:H | 14:YD:22[C]:ALA:HB3 | 1.60 | 0.64 |
| 2:Z:821:ILE:HG22 | 2:Z:822:ALA:H | 1.62 | 0.64 |
| 6:AF:39:THR:OG1 | 6:AF:42:GLN:OE1 | 2.14 | 0.64 |
| 6:AH:39:THR:OG1 | 6:AH:42:GLN:OE1 | 2.14 | 0.64 |
| 7:AI:476:ASP:O | 7:AI:479:ASN:ND2 | 2.31 | 0.64 |
| 7:AJ:146:SER:H | 7:AJ:149:GLN:HB2 | 1.61 | 0.64 |
| 7:BA:181:THR:O | 7:BA:190:VAL:N | 2.31 | 0.64 |
| 1:BI:361:GLN:HG2 | 1:BI:455:PHE:CE2 | 2.31 | 0.64 |
| 2:C:109:THR:OG1 | 2:C:624:GLN:NE2 | 2.31 | 0.64 |
| 3:CA:282:LYS:NZ | 3:CA:289:ASN:OD1 | 2.21 | 0.64 |
| 3:CB:292:ALA:HB1 | 3:CB:297:TYR:HE2 | 1.62 | 0.64 |
| 5:CF:164:ARG:HG3 | 5:CF:245:GLU:HG2 | 1.78 | 0.64 |
| 7:DB:496:ARG:NH1 | 7:DB:501:THR:OG1 | 2.29 | 0.64 |
| 1:EA:18:PRO:HG3 | 2:EC:701:TRP:CD1 | 2.32 | 0.64 |
| 1:EB:411:PRO:HG2 | 1:EB:413:TYR:CE1 | 2.32 | 0.64 |
| 6:FC:205:ASN:HB2 | 7:HI:175:GLN:O | 1.98 | 0.64 |
| 3:GG:304:ARG:HG2 | 3:GG:305:HIS:ND1 | 2.13 | 0.64 |
| 5:HC:186:TYR:HE1 | 5:HC:246:THR:HA | 1.63 | 0.64 |
| 5:HC:89:TYR:O | 5:HC:91:LYS:N | 2.30 | 0.64 |
| 7:HH:101:SER:HB3 | 7:HH:120:LYS:HE3 | 1.79 | 0.64 |
| 7:HH:143:LYS:HA | 7:HI:134:SER:HB2 | 1.79 | 0.64 |
| 7:HH:176:ILE:HG12 | 7:HH:177:ALA:H | 1.62 | 0.64 |
| 7:HJ:310:ASN:OD1 | 7:HJ:311:GLY:N | 2.31 | 0.64 |
| 5:I:312:ARG:O | 5:I:382:ASN:N | 2.24 | 0.64 |
| 5:J:329:PHE:HB3 | 5:J:332:VAL:HB | 1.79 | 0.64 |
| 5:J:89:TYR:O | 5:J:91:LYS:N | 2.30 | 0.64 |
| 7:Q:181:THR:O | 7:Q:190:VAL:N | 2.31 | 0.64 |
| 1:X:145:PHE:HB2 | 1:X:168:ALA:O | 1.97 | 0.64 |
| 13:YA:30[F]:ARG:HB2 | 13:YA:52[F]:LEU:HD21 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:434[F]:THR:OG1 | 13:YB:430[F]:ARG:NH1 | 2.30 | 0.64 |
| 13:YB:538[D]:VAL:HG11 | 13:YC:534[D]:LEU:HB2 | 1.78 | 0.64 |
| 13:YB:95[A]:ILE:HD11 | 13:YC:83[A]:TYR:CZ | 2.32 | 0.64 |
| 13:YC:30[B]:ARG:HB2 | 13:YC:52[B]:LEU:HD21 | 1.79 | 0.64 |
| 14:YD:312[F]:THR:OG1 | 14:YD:313[F]:ILE:N | 2.30 | 0.64 |
| 14:YD:312[D]:THR:OG1 | 14:YD:313[D]:ILE:N | 2.29 | 0.64 |
| 14:YE:312[C]:THR:OG1 | 14:YE:313[C]:ILE:N | 2.29 | 0.64 |
| 14:YF:125[A]:PHE:CE2 | 14:YF:134[A]:GLU:HG3 | 2.30 | 0.64 |
| 14:YF:288[B]:TYR:OH | 14:YF:371[B]:LYS:NZ | 2.27 | 0.64 |
| 1:A:543:THR:HG21 | 1:A:552:LYS:H | 1.62 | 0.64 |
| 5:AC:237:ASN:OD1 | 5:AC:238:ILE:N | 2.31 | 0.64 |
| 5:AD:117:ILE:HG22 | 5:AD:143:TRP:HE3 | 1.62 | 0.64 |
| 5:AD:312:ARG:HG2 | 5:AD:317:LEU:HA | 1.78 | 0.64 |
| 5:AE:158:ASP:O | 5:AE:161:ASN:N | 2.31 | 0.64 |
| 1:BH:396:LEU:O | 1:BH:399:TYR:N | 2.30 | 0.64 |
| 2:C:436:THR:HG22 | 2:C:441:VAL:HG12 | 1.79 | 0.64 |
| 2:C:81:ARG:HD2 | 2:C:94:TRP:HB3 | 1.77 | 0.64 |
| 2:C:925:LEU:HD12 | 2:C:993:LEU:HB3 | 1.80 | 0.64 |
| 3:CA:147:LEU:HD23 | 3:CA:149:ASP:H | 1.63 | 0.64 |
| 6:CI:77:VAL:HG23 | 7:FF:167:GLN:NE2 | 2.12 | 0.64 |
| 7:DD:497:ASN:H | 7:DD:500:TYR:HB2 | 1.62 | 0.64 |
| 1:EB:361:GLN:HG2 | 1:EB:455:PHE:CE2 | 2.31 | 0.64 |
| 5:EI:290:SER:HA | 5:EI:371:PHE:HB3 | 1.80 | 0.64 |
| 5:FA:555:CYS:O | 5:FA:556:GLN:HG2 | 1.97 | 0.64 |
| 7:FE:449:GLY:HA2 | 7:FF:484:THR:HG22 | 1.80 | 0.64 |
| 2:GF:232:PRO:HG3 | 2:GF:237:VAL:HG22 | 1.79 | 0.64 |
| 2:GF:423:GLU:OE1 | 2:GF:423:GLU:N | 2.30 | 0.64 |
| 1:GD:18:PRO:HG3 | 2:GF:701:TRP:CD1 | 2.32 | 0.64 |
| 3:GH:51:GLU:OE2 | 3:GH:270:ARG:NH2 | 2.29 | 0.64 |
| 5:HD:340:VAL:HG23 | 5:HD:341:GLU:HG3 | 1.79 | 0.64 |
| 6:HE:13:ARG:HD2 | 6:HG:10:VAL:HA | 1.78 | 0.64 |
| 12:IF:233:ASP:OD1 | 12:IF:234:ASN:N | 2.29 | 0.64 |
| 5:J:137:TYR:HA | 5:J:143:TRP:CD1 | 2.32 | 0.64 |
| 5:J:119:GLY:H | 5:J:142:ARG:HH22 | 1.44 | 0.64 |
| 5:K:292:PRO:HA | 5:K:368:ILE:HD12 | 1.80 | 0.64 |
| 6:M:16:ASP:OD2 | 6:M:45:LYS:NZ | 2.29 | 0.64 |
| 5:I:356:TYR:HE1 | 6:N:4:LEU:HD13 | 1.61 | 0.64 |
| 7:P:205:ARG:HH12 | 6:HE:218:THR:HB | 1.62 | 0.64 |
| 1:X:8:TYR:OH | 1:X:19:GLU:HG3 | 1.98 | 0.64 |
| 1:X:578:ASN:OD1 | 1:X:579:LYS:N | 2.30 | 0.64 |
| 13:YA:30[E]:ARG:HB2 | 13:YA:52[E]:LEU:HD21 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:38[B]:GLN:N | 13:YA:38[B]:GLN:OE1 | 2.30 | 0.64 |
| 13:YC:38[B]:GLN:N | 13:YC:38[B]:GLN:OE1 | 2.30 | 0.64 |
| 13:YC:47[F]:ILE:HG23 | 14:YF:123[F]:PRO:HG3 | 1.78 | 0.64 |
| 13:YA:72[E]:SER:O | 13:YC:61[E]:ILE:HD11 | 1.98 | 0.64 |
| 2:Z:67:PHE:HE2 | 2:Z:69:PHE:HB2 | 1.60 | 0.64 |
| 1:BH:649:GLN:OE1 | 1:BH:649:GLN:N | 2.25 | 0.64 |
| 5:CF:34:TYR:O | 5:CF:38:GLY:N | 2.26 | 0.64 |
| 5:CG:186:TYR:HE1 | 5:CG:246:THR:HA | 1.63 | 0.64 |
| 7:DB:143:LYS:HA | 7:DC:134:SER:HB2 | 1.80 | 0.64 |
| 1:EA:98:TYR:HB2 | 1:EA:332:LYS:HG2 | 1.80 | 0.64 |
| 3:ED:304:ARG:HG2 | 3:ED:305:HIS:ND1 | 2.13 | 0.64 |
| 4:EF:106:CYS:SG | 4:EF:149:ARG:NH2 | 2.67 | 0.64 |
| 5:EI:279:SER:HB2 | 5:FA:326:MET:HE3 | 1.79 | 0.64 |
| 5:EJ:186:TYR:HE1 | 5:EJ:246:THR:HA | 1.63 | 0.64 |
| 5:EJ:89:TYR:O | 5:EJ:91:LYS:N | 2.30 | 0.64 |
| 5:FA:195:HIS:N | 5:FA:197:GLY:O | 2.31 | 0.64 |
| 5:EI:251:VAL:HG11 | 5:FA:254:TRP:CZ2 | 2.32 | 0.64 |
| 5:FA:312:ARG:HD3 | 5:FA:317:LEU:HD12 | 1.80 | 0.64 |
| 7:FF:481:SER:OG | 7:FG:449:GLY:O | 2.16 | 0.64 |
| 7:FG:181:THR:O | 7:FG:190:VAL:N | 2.31 | 0.64 |
| 7:FG:310:ASN:OD1 | 7:FG:311:GLY:N | 2.31 | 0.64 |
| 2:EC:664:PHE:HB2 | 9:FJ:15:MET:HB2 | 1.80 | 0.64 |
| 2:GF:109:THR:OG1 | 2:GF:624:GLN:NE2 | 2.31 | 0.64 |
| 5:HD:312:ARG:HD3 | 5:HD:317:LEU:HD12 | 1.80 | 0.64 |
| 5:I:237:ASN:OD1 | 5:I:238:ILE:N | 2.31 | 0.64 |
| 5:I:387:ASN:HB3 | 5:I:389:ASP:OD1 | 1.98 | 0.64 |
| 12:IF:15:ASP:CG | 12:IF:16:PHE:H | 2.00 | 0.64 |
| 5:K:312:ARG:HD3 | 5:K:317:LEU:HD12 | 1.80 | 0.64 |
| 7:O:193:LEU:HD13 | 7:P:206:GLU:HG3 | 1.80 | 0.64 |
| 9:T:20:ASN:OD1 | 12:BG:233:ASP:HA | 109.54 | 0.64 |
| 12:W:233:ASP:OD1 | 12:W:234:ASN:N | 2.29 | 0.64 |
| 13:YB:232[A]:ASN:CB | 13:YC:407[A]:PRO:HB3 | 2.27 | 0.64 |
| 13:YB:38[A]:GLN:N | 13:YB:38[A]:GLN:OE1 | 2.30 | 0.64 |
| 13:YB:418[F]:THR:HG21 | 13:YC:428[F]:GLY:HA3 | 1.79 | 0.64 |
| 13:YB:30[C]:ARG:HB2 | 13:YB:52[C]:LEU:HD21 | 1.79 | 0.64 |
| 13:YB:538[F]:VAL:HG11 | 13:YC:534[F]:LEU:HB2 | 1.79 | 0.64 |
| 13:YA:551[D]:THR:HG22 | 13:YC:558[D]:SER:HB3 | 1.78 | 0.64 |
| 2:Z:109:THR:OG1 | 2:Z:624:GLN:NE2 | 2.31 | 0.64 |
| 2:Z:849:GLN:HG3 | 2:Z:852:ILE:HD12 | 1.80 | 0.64 |
| 5:AC:102:TRP:CE3 | 5:AC:131:SER:HB2 | 2.32 | 0.64 |
| 5:AD:175:THR:O | 5:AD:232:LEU:N | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:193:LEU:HD21 | 7:BA:207:GLY:HA2 | 1.80 | 0.64 |
| 2:BJ:1014:ASP:HA | 2:BJ:1027:GLN:HB3 | 1.79 | 0.64 |
| 2:BJ:1012:LEU:HD13 | 2:BJ:1027:GLN:CD | 2.18 | 0.64 |
| 2:C:821:ILE:C | 2:C:824:GLN:HE22 | 2.01 | 0.64 |
| 2:C:33:TYR:HB3 | 3:D:156:LEU:HD22 | 1.80 | 0.64 |
| 3:D:304:ARG:HG2 | 3:D:305:HIS:ND1 | 2.13 | 0.64 |
| 7:DD:181:THR:O | 7:DD:190:VAL:N | 2.31 | 0.64 |
| 8:BC:43:ALA:CB | 8:DF:138:GLY:HA3 | 2.28 | 0.64 |
| 1:EA:34:ILE:HG23 | 1:EA:48:PHE:HD2 | 1.62 | 0.64 |
| 2:EC:134:TYR:OH | 2:EC:593:GLU:HG2 | 1.97 | 0.64 |
| 2:EC:81:ARG:HG2 | 2:EC:94:TRP:HE3 | 1.63 | 0.64 |
| 2:EC:884:HIS:ND1 | 2:EC:885:PRO:O | 2.29 | 0.64 |
| 3:ED:270:ARG:CZ | 3:ED:317:PRO:HB3 | 2.28 | 0.64 |
| 5:FA:312:ARG:O | 5:FA:382:ASN:N | 2.25 | 0.64 |
| 6:FD:16:ASP:OD2 | 6:FD:45:LYS:NZ | 2.29 | 0.64 |
| 7:FF:453:GLU:OE2 | 7:FF:471:THR:N | 2.31 | 0.64 |
| 9:FJ:89:ASP:HB2 | 9:FJ:113:ILE:HD13 | 1.80 | 0.64 |
| 1:GD:156:ASP:OD1 | 1:GD:157:LYS:N | 2.29 | 0.64 |
| 1:GD:98:TYR:HB2 | 1:GD:332:LYS:HG2 | 1.80 | 0.64 |
| 2:GF:68:PHE:CZ | 2:GF:564:GLY:HA2 | 2.32 | 0.64 |
| 3:GG:147:LEU:HD23 | 3:GG:149:ASP:H | 1.63 | 0.64 |
| 5:HB:102:TRP:CE3 | 5:HB:131:SER:HB2 | 2.32 | 0.64 |
| 5:HB:387:ASN:HB3 | 5:HB:389:ASP:OD1 | 1.98 | 0.64 |
| 8:FH:43:ALA:HB1 | 8:IA:138:GLY:HA3 | 1.80 | 0.64 |
| 7:Q:365:GLY:HA2 | 7:HI:71:ASN:CB | 2.27 | 0.64 |
| 13:YB:232[B]:ASN:CB | 13:YC:407[B]:PRO:HB3 | 2.27 | 0.64 |
| 13:YA:551[C]:THR:HG22 | 13:YC:558[C]:SER:HB3 | 1.78 | 0.64 |
| 13:YA:76[D]:PRO:CA | 13:YC:61[D]:ILE:HA | 2.26 | 0.64 |
| 14:YF:312[F]:THR:OG1 | 14:YF:313[F]:ILE:N | 2.30 | 0.64 |
| 2:Z:423:GLU:OE1 | 2:Z:423:GLU:N | 2.30 | 0.64 |
| 5:AC:290:SER:HA | 5:AC:371:PHE:HB3 | 1.80 | 0.64 |
| 5:AC:62:ALA:HB1 | 5:AC:82:PRO:HG3 | 1.80 | 0.64 |
| 5:AE:316:ILE:HG22 | 5:AE:318:GLN:HG3 | 1.78 | 0.64 |
| 7:AI:212:PRO:HB3 | 7:AJ:199:VAL:HA | 1.78 | 0.64 |
| 2:BJ:186:ASP:OD1 | 2:BJ:187:ILE:N | 2.31 | 0.64 |
| 2:BJ:884:HIS:ND1 | 2:BJ:885:PRO:O | 2.30 | 0.64 |
| 2:C:821:ILE:HG22 | 2:C:822:ALA:H | 1.62 | 0.64 |
| 5:CF:290:SER:HA | 5:CF:371:PHE:HB3 | 1.80 | 0.64 |
| 5:CF:263:ILE:HG22 | 5:CF:381:ILE:HB | 1.79 | 0.64 |
| 5:CH:196:ARG:NH1 | 7:DC:5:THR:O | 2.31 | 0.64 |
| 8:DF:43:ALA:CB | 8:FI:138:GLY:HA3 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:84:ASN:ND2 | 11:DI:14:LYS:O | 2.31 | 0.64 |
| 11:DI:2:LEU:HD11 | 11:DI:71:TRP:CD2 | 2.33 | 0.64 |
| 1:EA:7:ASN:HD22 | 2:EC:634:PRO:HG2 | 1.61 | 0.64 |
| 1:EA:8:TYR:OH | 1:EA:19:GLU:HG3 | 1.98 | 0.64 |
| 2:EC:1012:LEU:HD13 | 2:EC:1027:GLN:CD | 2.18 | 0.64 |
| 5:EI:312:ARG:O | 5:EI:382:ASN:N | 2.24 | 0.64 |
| 7:FG:177:ALA:HB3 | 7:FG:178:PRO:HD3 | 1.78 | 0.64 |
| 1:GD:566:ASN:OD1 | 1:GD:567:GLU:N | 2.31 | 0.64 |
| 2:GF:186:ASP:OD1 | 2:GF:187:ILE:N | 2.31 | 0.64 |
| 2:GF:821:ILE:C | 2:GF:824:GLN:HE22 | 2.01 | 0.64 |
| 4:GI:106:CYS:SG | 4:GI:149:ARG:NH2 | 2.67 | 0.64 |
| 5:HB:38:GLY:HA2 | 5:HB:43:PRO:HA | 1.80 | 0.64 |
| 7:HJ:145:SER:O | 7:HJ:164:LYS:NZ | 2.25 | 0.64 |
| 5:I:290:SER:HA | 5:I:371:PHE:HB3 | 1.80 | 0.64 |
| 5:J:103:ASN:N | 5:J:127:ASN:O | 2.31 | 0.64 |
| 5:J:186:TYR:HE1 | 5:J:246:THR:HA | 1.63 | 0.64 |
| 7:P:81:LEU:O | 7:P:85:LEU:N | 2.30 | 0.64 |
| 1:X:396:LEU:O | 1:X:399:TYR:N | 2.30 | 0.64 |
| 13:YA:434[D]:THR:OG1 | 13:YB:430[D]:ARG:NH1 | 2.31 | 0.64 |
| 13:YB:232[E]:ASN:CB | 13:YC:407[E]:PRO:HB3 | 2.27 | 0.64 |
| 13:YC:38[C]:GLN:N | 13:YC:38[C]:GLN:OE1 | 2.29 | 0.64 |
| 2:Z:788:THR:HG23 | 2:Z:790:THR:H | 1.63 | 0.64 |
| 1:A:424:TYR:HE2 | 1:A:655:LEU:HD13 | 1.63 | 0.64 |
| 5:AE:312:ARG:HD3 | 5:AE:317:LEU:HD12 | 1.80 | 0.64 |
| 1:BH:98:TYR:HB2 | 1:BH:332:LYS:HG2 | 1.80 | 0.64 |
| 2:BJ:109:THR:OG1 | 2:BJ:624:GLN:NE2 | 2.31 | 0.64 |
| 2:BJ:788:THR:HG23 | 2:BJ:790:THR:H | 1.63 | 0.64 |
| 5:CF:102:TRP:CE3 | 5:CF:131:SER:HB2 | 2.32 | 0.64 |
| 5:CH:312:ARG:HD3 | 5:CH:317:LEU:HD12 | 1.80 | 0.64 |
| 7:DD:310:ASN:OD1 | 7:DD:311:GLY:N | 2.31 | 0.64 |
| 1:EA:257:ILE:HG12 | 1:EB:331:ILE:HD11 | 1.80 | 0.64 |
| 5:EI:102:TRP:CE3 | 5:EI:131:SER:HB2 | 2.32 | 0.64 |
| 5:EJ:71:ASN:OD1 | 5:EJ:73:SER:N | 2.23 | 0.64 |
| 1:GD:145:PHE:HB2 | 1:GD:168:ALA:O | 1.97 | 0.64 |
| 3:GH:292:ALA:HB1 | 3:GH:297:TYR:CE2 | 2.33 | 0.64 |
| 5:J:320:LEU:HG | 5:J:357:SER:HB3 | 1.80 | 0.64 |
| 5:I:241:THR:HG21 | 5:K:200:LEU:HD13 | 1.79 | 0.64 |
| 6:L:12:SER:HB3 | 6:N:6:ASN:HB3 | 1.79 | 0.64 |
| 7:O:476:ASP:O | 7:O:479:ASN:ND2 | 2.31 | 0.64 |
| 7:P:453:GLU:OE2 | 7:P:471:THR:N | 2.31 | 0.64 |
| 7:O:77:THR:HG21 | 7:P:72:ASN:HA | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:18:PRO:HG3 | 2:Z:701:TRP:CD1 | 2.33 | 0.64 |
| 1:X:522:LYS:HA | 1:X:534:VAL:HG23 | 1.78 | 0.64 |
| 1:Y:148:ARG:HH22 | 1:Y:196:GLN:HE22 | 1.46 | 0.64 |
| 13:YB:193[C]:ASP:OD1 | 13:YB:197[C]:TYR:N | 2.31 | 0.64 |
| 13:YB:38[E]:GLN:OE1 | 13:YB:38[E]:GLN:N | 2.30 | 0.64 |
| 13:YA:434[C]:THR:OG1 | 13:YB:430[C]:ARG:NH1 | 2.30 | 0.64 |
| 13:YC:30[A]:ARG:HB2 | 13:YC:52[A]:LEU:HD21 | 1.79 | 0.64 |
| 13:YC:38[E]:GLN:N | 13:YC:38[E]:GLN:OE1 | 2.30 | 0.64 |
| 14:YD:312[E]:THR:OG1 | 14:YD:313[E]:ILE:N | 2.30 | 0.64 |
| 11:DI:178:ASN:N | 14:YF:217[F]:SER:O | 2.29 | 0.64 |
| 14:YF:312[C]:THR:OG1 | 14:YF:313[C]:ILE:N | 2.29 | 0.64 |
| 2:Z:821:ILE:C | 2:Z:824:GLN:HE22 | 2.01 | 0.64 |
| 2:Z:884:HIS:ND1 | 2:Z:885:PRO:O | 2.29 | 0.64 |
| 2:Z:981:GLN:N | 2:Z:981:GLN:OE1 | 2.29 | 0.64 |
| 5:AC:111:ALA:HB2 | 5:AC:117:ILE:HG23 | 1.80 | 0.64 |
| 5:AC:206:PHE:HZ | 5:AC:221:GLU:HG2 | 1.63 | 0.64 |
| 5:AD:103:ASN:N | 5:AD:127:ASN:O | 2.31 | 0.64 |
| 7:AI:330:ARG:NH2 | 7:AI:336:GLU:OE2 | 2.27 | 0.64 |
| 1:B:553:VAL:N | 1:B:593:GLY:O | 2.23 | 0.64 |
| 9:BD:89:ASP:HB2 | 9:BD:113:ILE:HD13 | 1.80 | 0.64 |
| 1:BH:539:ARG:HD3 | 1:BH:580:LEU:HB3 | 1.80 | 0.64 |
| 2:BJ:928:GLU:OE2 | 2:BJ:960:GLY:HA2 | 1.98 | 0.64 |
| 2:C:326:VAL:HG21 | 2:C:413:TRP:HZ2 | 1.63 | 0.64 |
| 2:C:849:GLN:HG3 | 2:C:852:ILE:HD12 | 1.80 | 0.64 |
| 5:CF:206:PHE:HZ | 5:CF:221:GLU:HG2 | 1.63 | 0.64 |
| 7:DB:476:ASP:O | 7:DB:479:ASN:ND2 | 2.31 | 0.64 |
| 8:BB:162:TRP:O | 8:DE:95:GLN:NE2 | 2.31 | 0.64 |
| 9:DG:89:ASP:HB2 | 9:DG:113:ILE:HD13 | 1.80 | 0.64 |
| 1:EA:566:ASN:OD1 | 1:EA:567:GLU:N | 2.31 | 0.64 |
| 1:EB:155:ARG:HA | 1:EB:161:TYR:HB3 | 1.80 | 0.64 |
| 2:EC:584:GLY:HA3 | 2:EC:597:TYR:OH | 1.98 | 0.64 |
| 5:EI:107:VAL:O | 5:EI:125:GLU:HG3 | 1.98 | 0.64 |
| 5:EJ:137:TYR:HA | 5:EJ:143:TRP:CD1 | 2.32 | 0.64 |
| 6:FC:52:ILE:HD11 | 6:FD:15:ALA:HB2 | 1.80 | 0.64 |
| 7:FG:67:ILE:HA | 7:FG:84:ARG:HH21 | 1.62 | 0.64 |
| 11:GB:2:LEU:HD11 | 11:GB:71:TRP:CD2 | 2.33 | 0.64 |
| 1:GD:337:GLN:HG3 | 1:GE:334:GLU:HG2 | 1.80 | 0.64 |
| 1:GD:510:MET:HB3 | 1:GD:542:SER:HB3 | 1.79 | 0.64 |
| 1:GD:539:ARG:HD3 | 1:GD:580:LEU:HB3 | 1.80 | 0.64 |
| 2:GF:584:GLY:HA3 | 2:GF:597:TYR:OH | 1.98 | 0.64 |
| 2:GF:849:GLN:HG3 | 2:GF:852:ILE:HD12 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:42:GLY:HA2 | 3:GH:76:MET:HG2 | 1.79 | 0.64 |
| 5:HD:158:ASP:O | 5:HD:161:ASN:N | 2.31 | 0.64 |
| 5:HD:292:PRO:HA | 5:HD:368:ILE:HD12 | 1.80 | 0.64 |
| 6:HF:17:PHE:O | 6:HG:13:ARG:NH1 | 2.21 | 0.64 |
| 8:R:79:HIS:HB2 | 8:IA:125:LYS:HG2 | 1.80 | 0.64 |
| 12:IF:216:PHE:HE1 | 12:IF:218:MET:HE3 | 1.62 | 0.64 |
| 9:T:98:VAL:N | 9:T:103:THR:O | 2.26 | 0.64 |
| 1:Y:411:PRO:HG2 | 1:Y:413:TYR:CE1 | 2.32 | 0.64 |
| 13:YA:38[A]:GLN:OE1 | 13:YA:38[A]:GLN:N | 2.30 | 0.64 |
| 13:YB:30[D]:ARG:HB2 | 13:YB:52[D]:LEU:HD21 | 1.79 | 0.64 |
| 13:YA:434[E]:THR:OG1 | 13:YB:430[E]:ARG:NH1 | 2.31 | 0.64 |
| 14:YF:312[A]:THR:OG1 | 14:YF:313[A]:ILE:N | 2.30 | 0.64 |
| 2:Z:186:ASP:OD1 | 2:Z:187:ILE:N | 2.31 | 0.64 |
| 2:Z:993:LEU:HD12 | 2:Z:995:ASP:H | 1.63 | 0.64 |
| 5:AE:214:SER:OG | 5:AE:222:LEU:O | 2.16 | 0.63 |
| 1:BH:543:THR:HG21 | 1:BH:552:LYS:H | 1.62 | 0.63 |
| 2:BJ:436:THR:HG22 | 2:BJ:441:VAL:HG12 | 1.79 | 0.63 |
| 2:BJ:68:PHE:CZ | 2:BJ:564:GLY:HA2 | 2.32 | 0.63 |
| 2:C:423:GLU:N | 2:C:423:GLU:OE1 | 2.30 | 0.63 |
| 2:C:117:GLN:O | 2:C:596:SER:OG | 2.15 | 0.63 |
| 3:CA:304:ARG:HG2 | 3:CA:305:HIS:ND1 | 2.13 | 0.63 |
| 5:CF:187:ASN:HB2 | 5:CF:254:TRP:HZ2 | 1.63 | 0.63 |
| 5:CG:117:ILE:HG22 | 5:CG:143:TRP:HE3 | 1.62 | 0.63 |
| 5:CH:195:HIS:N | 5:CH:197:GLY:O | 2.30 | 0.63 |
| 5:CH:312:ARG:O | 5:CH:382:ASN:N | 2.25 | 0.63 |
| 5:CH:555:CYS:O | 5:CH:556:GLN:HG2 | 1.97 | 0.63 |
| 3:D:147:LEU:HD23 | 3:D:149:ASP:H | 1.63 | 0.63 |
| 7:DC:214:THR:HA | 7:DC:217:ASN:ND2 | 2.13 | 0.63 |
| 3:E:292:ALA:HB1 | 3:E:297:TYR:CE2 | 2.33 | 0.63 |
| 5:EJ:117:ILE:HG22 | 5:EJ:143:TRP:HE3 | 1.62 | 0.63 |
| 5:FA:158:ASP:O | 5:FA:161:ASN:N | 2.31 | 0.63 |
| 5:FA:313:PHE:HE1 | 6:FC:8:ALA:HB1 | 1.61 | 0.63 |
| 5:AE:362:GLU:OE2 | 7:FE:473:LYS:HE2 | 1.98 | 0.63 |
| 4:G:43:GLY:O | 4:G:68:GLN:NE2 | 2.32 | 0.63 |
| 5:HB:187:ASN:HB2 | 5:HB:254:TRP:HZ2 | 1.63 | 0.63 |
| 5:HB:290:SER:HA | 5:HB:371:PHE:HB3 | 1.80 | 0.63 |
| 5:HC:71:ASN:OD1 | 5:HC:73:SER:N | 2.23 | 0.63 |
| 5:HC:36:GLU:HG3 | 5:HD:43:PRO:HG2 | 1.78 | 0.63 |
| 6:HE:60:HIS:NE2 | 6:HG:28:ASP:OD2 | 2.31 | 0.63 |
| 5:I:164:ARG:HG3 | 5:I:245:GLU:HG2 | 1.78 | 0.63 |
| 5:I:206:PHE:HZ | 5:I:221:GLU:HG2 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:187:ASN:HB2 | 5:I:254:TRP:HZ2 | 1.64 | 0.63 |
| 7:O:101:SER:HB3 | 7:O:120:LYS:HE3 | 1.79 | 0.63 |
| 7:O:176:ILE:HG12 | 7:O:177:ALA:H | 1.61 | 0.63 |
| 9:T:85:GLU:OE2 | 9:T:87:ARG:NE | 2.29 | 0.63 |
| 11:V:2:LEU:HD11 | 11:V:71:TRP:CD2 | 2.33 | 0.63 |
| 12:W:168:ALA:N | 12:IF:211:HIS:HE1 | 1.93 | 0.63 |
| 1:X:358:GLN:HB2 | 1:X:379:LYS:HB3 | 1.80 | 0.63 |
| 1:X:337:GLN:HG3 | 1:Y:334:GLU:HG2 | 1.79 | 0.63 |
| 13:YA:30[C]:ARG:HB2 | 13:YA:52[C]:LEU:HD21 | 1.79 | 0.63 |
| 13:YB:563[A]:GLY:N | 13:YC:555[A]:ALA:O | 2.30 | 0.63 |
| 11:DI:178:ASN:N | 14:YE:217[B]:SER:O | 2.29 | 0.63 |
| 2:Z:1014:ASP:HA | 2:Z:1027:GLN:HB3 | 1.80 | 0.63 |
| 2:Z:117:GLN:O | 2:Z:596:SER:OG | 2.15 | 0.63 |
| 1:A:566:ASN:OD1 | 1:A:567:GLU:N | 2.31 | 0.63 |
| 7:AI:449:GLY:HA2 | 7:AJ:484:THR:HG22 | 1.80 | 0.63 |
| 1:B:543:THR:OG1 | 1:B:544:ASP:N | 2.29 | 0.63 |
| 1:BH:18:PRO:HG3 | 2:BJ:701:TRP:CD1 | 2.33 | 0.63 |
| 1:BH:553:VAL:N | 1:BH:593:GLY:O | 2.21 | 0.63 |
| 1:BI:214:MET:N | 2:BJ:733:ASP:OD2 | 2.31 | 0.63 |
| 2:C:513:PHE:HB3 | 2:C:525:TRP:CZ3 | 2.33 | 0.63 |
| 5:CF:237:ASN:OD1 | 5:CF:238:ILE:N | 2.31 | 0.63 |
| 7:DC:211:SER:H | 7:DC:214:THR:HG1 | 1.44 | 0.63 |
| 1:EA:539:ARG:HD3 | 1:EA:580:LEU:HB3 | 1.80 | 0.63 |
| 1:EA:424:TYR:HE2 | 1:EA:655:LEU:HD13 | 1.63 | 0.63 |
| 4:EF:282:GLN:NE2 | 4:EH:275:ALA:O | 2.31 | 0.63 |
| 5:EJ:36:GLU:HG3 | 5:FA:43:PRO:HG2 | 1.79 | 0.63 |
| 7:FE:498:SER:O | 7:FG:422:LYS:NZ | 2.31 | 0.63 |
| 1:GD:257:ILE:HG12 | 1:GE:331:ILE:HD11 | 1.80 | 0.63 |
| 1:GE:521:ARG:O | 1:GE:533:ASP:HB2 | 1.97 | 0.63 |
| 3:GH:226:GLU:N | 3:GH:226:GLU:OE1 | 2.31 | 0.63 |
| 4:H:106:CYS:SG | 4:H:149:ARG:NH2 | 2.67 | 0.63 |
| 5:HB:154:ILE:HG12 | 5:HC:153:LYS:HZ2 | 1.63 | 0.63 |
| 5:HC:253:GLN:HE22 | 5:HD:249:ASP:HB3 | 1.63 | 0.63 |
| 5:HC:320:LEU:HG | 5:HC:357:SER:HB3 | 1.80 | 0.63 |
| 6:HE:16:ASP:OD2 | 6:HE:45:LYS:NZ | 2.29 | 0.63 |
| 7:HH:289:GLN:HA | 7:HI:287:VAL:HA | 1.79 | 0.63 |
| 7:HH:77:THR:HG21 | 7:HI:72:ASN:HA | 1.80 | 0.63 |
| 10:U:349:ARG:HD3 | 10:ID:143:PHE:CD2 | 2.34 | 0.63 |
| 10:ID:285:LEU:HA | 14:YE:215[D]:GLU:CG | 2.29 | 0.63 |
| 5:J:317:LEU:HD13 | 5:K:312:ARG:HH22 | 1.63 | 0.63 |
| 5:J:71:ASN:OD1 | 5:J:73:SER:N | 2.23 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:218:SER:O | 7:P:227:VAL:HG22 | 1.98 | 0.63 |
| 7:P:509:GLY:HA3 | 7:Q:441:GLN:HE21 | 1.61 | 0.63 |
| 1:X:517:PHE:N | 1:X:536:TYR:O | 2.24 | 0.63 |
| 1:Y:155:ARG:HA | 1:Y:161:TYR:HB3 | 1.81 | 0.63 |
| 13:YA:434[A]:THR:OG1 | 13:YB:430[A]:ARG:NH1 | 2.31 | 0.63 |
| 13:YA:533[F]:ASN:HD22 | 13:YC:540[F]:GLY:HA3 | 1.62 | 0.63 |
| 13:YB:538[A]:VAL:HG11 | 13:YC:534[A]:LEU:HB2 | 1.79 | 0.63 |
| 13:YB:563[B]:GLY:N | 13:YC:555[B]:ALA:O | 2.29 | 0.63 |
| 13:YC:24[D]:LEU:HD23 | 14:YF:259[D]:LEU:HD22 | 1.80 | 0.63 |
| 13:YB:418[C]:THR:HG21 | 13:YC:428[C]:GLY:HA3 | 1.79 | 0.63 |
| 13:YB:442[C]:THR:HA | 13:YC:434[C]:THR:O | 1.99 | 0.63 |
| 13:YB:442[F]:THR:HA | 13:YC:434[F]:THR:O | 1.99 | 0.63 |
| 13:YC:47[E]:ILE:HG23 | 14:YF:123[E]:PRO:HG3 | 1.79 | 0.63 |
| 13:YA:533[A]:ASN:HD22 | 13:YC:540[A]:GLY:HA3 | 1.62 | 0.63 |
| 13:YC:24[A]:LEU:HD23 | 14:YF:259[A]:LEU:HD22 | 1.80 | 0.63 |
| 14:YF:288[A]:TYR:OH | 14:YF:371[A]:LYS:NZ | 2.27 | 0.63 |
| 1:BH:8:TYR:OH | 1:BH:19:GLU:HG3 | 1.98 | 0.63 |
| 2:BJ:821:ILE:HG22 | 2:BJ:822:ALA:H | 1.62 | 0.63 |
| 2:C:81:ARG:HG2 | 2:C:94:TRP:HE3 | 1.63 | 0.63 |
| 2:BJ:33:TYR:HB3 | 3:CA:156:LEU:HD22 | 1.79 | 0.63 |
| 5:CF:62:ALA:HB1 | 5:CF:82:PRO:HG3 | 1.80 | 0.63 |
| 5:CH:305:ASN:HB3 | 5:CH:388:ASN:HB2 | 1.79 | 0.63 |
| 7:DB:212:PRO:HB3 | 7:DC:199:VAL:HA | 1.80 | 0.63 |
| 7:DB:211:SER:N | 7:DB:214:THR:OG1 | 2.28 | 0.63 |
| 9:DG:98:VAL:N | 9:DG:103:THR:O | 2.26 | 0.63 |
| 10:BE:143:PHE:CD2 | 10:DH:349:ARG:HD3 | 2.32 | 0.63 |
| 2:C:897:THR:HG22 | 3:E:329:ASN:HB2 | 1.79 | 0.63 |
| 1:EA:578:ASN:OD1 | 1:EA:579:LYS:N | 2.30 | 0.63 |
| 1:EB:386:THR:OG1 | 1:EB:390:GLU:OE2 | 2.17 | 0.63 |
| 1:EB:543:THR:OG1 | 1:EB:544:ASP:N | 2.29 | 0.63 |
| 2:EC:109:THR:OG1 | 2:EC:624:GLN:NE2 | 2.31 | 0.63 |
| 7:FE:399:PHE:CD2 | 7:FG:514:PRO:HG2 | 2.34 | 0.63 |
| 7:FE:170:ILE:HD13 | 7:FF:172:LEU:HD22 | 1.79 | 0.63 |
| 7:FF:509:GLY:HA3 | 7:FG:441:GLN:HE21 | 1.63 | 0.63 |
| 12:GC:15:ASP:CG | 12:GC:16:PHE:H | 2.00 | 0.63 |
| 1:GD:649:GLN:OE1 | 1:GD:649:GLN:N | 2.25 | 0.63 |
| 5:HB:13:ASP:OD1 | 5:HB:14:GLY:N | 2.32 | 0.63 |
| 5:HB:264:ARG:HB3 | 5:HD:326:MET:HE1 | 1.79 | 0.63 |
| 5:HC:594:THR:HB | 5:HD:490:TRP:HB2 | 1.78 | 0.63 |
| 5:HD:305:ASN:HB3 | 5:HD:388:ASN:HB2 | 1.79 | 0.63 |
| 7:HH:418:ASP:OD1 | 7:HH:422:LYS:N | 2.30 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:248:MET:HB2 | 5:I:254:TRP:NE1 | 2.13 | 0.63 |
| 5:I:38:GLY:HA2 | 5:I:43:PRO:HA | 1.80 | 0.63 |
| 5:I:577:ASN:ND2 | 5:J:529:ASN:OD1 | 2.23 | 0.63 |
| 13:YC:30[E]:ARG:HB2 | 13:YC:52[E]:LEU:HD21 | 1.79 | 0.63 |
| 13:YB:575[D]:GLY:N | 13:YC:567[D]:ILE:O | 2.31 | 0.63 |
| 13:YC:87[D]:LEU:HD21 | 13:YC:95[D]:ILE:HG23 | 1.80 | 0.63 |
| 14:YF:305[B]:ASP:N | 14:YF:305[B]:ASP:OD1 | 2.31 | 0.63 |
| 1:A:517:PHE:N | 1:A:536:TYR:O | 2.24 | 0.63 |
| 5:AC:187:ASN:HB2 | 5:AC:254:TRP:HZ2 | 1.63 | 0.63 |
| 5:AC:387:ASN:HB3 | 5:AC:389:ASP:OD1 | 1.98 | 0.63 |
| 5:AD:371:PHE:CZ | 5:AD:373:SER:HB3 | 2.34 | 0.63 |
| 1:B:492:TYR:HA | 1:B:606:ILE:HD12 | 1.81 | 0.63 |
| 11:BF:131:TYR:O | 11:BF:148:GLY:N | 2.25 | 0.63 |
| 2:C:180:ILE:HG13 | 2:C:526:ILE:HD11 | 1.81 | 0.63 |
| 2:C:788:THR:HG23 | 2:C:790:THR:H | 1.63 | 0.63 |
| 5:CF:107:VAL:O | 5:CF:125:GLU:HG3 | 1.99 | 0.63 |
| 5:CF:38:GLY:HA2 | 5:CF:43:PRO:HA | 1.80 | 0.63 |
| 5:CG:212:PHE:HZ | 5:CG:230:ILE:HB | 1.64 | 0.63 |
| 3:D:47:TRP:CZ3 | 3:D:270:ARG:HD3 | 2.34 | 0.63 |
| 7:DB:86:SER:HA | 7:DB:97:LEU:HD12 | 1.79 | 0.63 |
| 2:EC:821:ILE:HG22 | 2:EC:822:ALA:H | 1.62 | 0.63 |
| 3:ED:44:SER:O | 3:ED:270:ARG:NH1 | 2.31 | 0.63 |
| 5:EI:237:ASN:OD1 | 5:EI:238:ILE:N | 2.31 | 0.63 |
| 5:EI:187:ASN:HB2 | 5:EI:254:TRP:HZ2 | 1.63 | 0.63 |
| 7:FE:289:GLN:HA | 7:FF:287:VAL:HA | 1.79 | 0.63 |
| 2:GF:821:ILE:HG22 | 2:GF:822:ALA:H | 1.62 | 0.63 |
| 2:GF:3:VAL:O | 2:GF:90:GLU:N | 2.26 | 0.63 |
| 3:GG:270:ARG:CZ | 3:GG:317:PRO:HB3 | 2.28 | 0.63 |
| 4:HA:43:GLY:O | 4:HA:68:GLN:NE2 | 2.32 | 0.63 |
| 5:HB:248:MET:HB2 | 5:HB:254:TRP:NE1 | 2.13 | 0.63 |
| 5:HB:472:TYR:HA | 5:HC:416:ILE:HG23 | 1.80 | 0.63 |
| 5:HC:196:ARG:HE | 7:HJ:5:THR:HG23 | 1.64 | 0.63 |
| 5:HD:195:HIS:N | 5:HD:197:GLY:O | 2.31 | 0.63 |
| 5:HB:409:SER:N | 5:HD:444:ASN:O | 2.30 | 0.63 |
| 7:HH:449:GLY:HA2 | 7:HI:484:THR:HG22 | 1.80 | 0.63 |
| 7:HJ:181:THR:O | 7:HJ:190:VAL:N | 2.31 | 0.63 |
| 11:IE:112:HIS:HB3 | 11:IE:150:LEU:HD13 | 1.81 | 0.63 |
| 5:K:313:PHE:HE1 | 6:M:8:ALA:HB1 | 1.63 | 0.63 |
| 1:X:34:ILE:HG23 | 1:X:48:PHE:HD2 | 1.62 | 0.63 |
| 1:X:510:MET:HB3 | 1:X:542:SER:HB3 | 1.79 | 0.63 |
| 13:YA:434[B]:THR:OG1 | 13:YB:430[B]:ARG:NH1 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:418[B]:THR:HG21 | 13:YC:428[B]:GLY:HA3 | 1.79 | 0.63 |
| 13:YB:418[D]:THR:HG21 | 13:YC:428[D]:GLY:HA3 | 1.80 | 0.63 |
| 13:YB:442[B]:THR:HA | 13:YC:434[B]:THR:O | 1.99 | 0.63 |
| 13:YB:563[C]:GLY:N | 13:YC:555[C]:ALA:O | 2.30 | 0.63 |
| 13:YB:575[B]:GLY:N | 13:YC:567[B]:ILE:O | 2.32 | 0.63 |
| 13:YC:87[C]:LEU:HD21 | 13:YC:95[C]:ILE:HG23 | 1.80 | 0.63 |
| 14:YD:211[F]:MET:HE1 | 14:YD:231[F]:ALA:HB2 | 1.78 | 0.63 |
| 14:YD:262[D]:SER:O | 14:YD:289[D]:ARG:NH1 | 2.32 | 0.63 |
| 14:YE:262[E]:SER:O | 14:YE:289[E]:ARG:NH1 | 2.32 | 0.63 |
| 14:YE:305[C]:ASP:OD1 | 14:YE:305[C]:ASP:N | 2.31 | 0.63 |
| 14:YE:312[E]:THR:OG1 | 14:YE:313[E]:ILE:N | 2.30 | 0.63 |
| 14:YF:305[A]:ASP:OD1 | 14:YF:305[A]:ASP:N | 2.31 | 0.63 |
| 2:Z:872:SER:O | 2:Z:873:SER:OG | 2.16 | 0.63 |
| 5:AC:304:ILE:HG23 | 5:AC:365:ILE:HD12 | 1.80 | 0.63 |
| 5:AD:212:PHE:HZ | 5:AD:230:ILE:HB | 1.63 | 0.63 |
| 6:AG:16:ASP:OD2 | 6:AG:45:LYS:NZ | 2.29 | 0.63 |
| 7:AI:303:GLU:HA | 7:AJ:309:ALA:HB3 | 1.80 | 0.63 |
| 7:AJ:100:TYR:OH | 7:BA:113:GLU:O | 2.05 | 0.63 |
| 11:BF:112:HIS:HB3 | 11:BF:150:LEU:HD13 | 1.81 | 0.63 |
| 2:BJ:872:SER:N | 2:BJ:894:THR:HG21 | 2.11 | 0.63 |
| 2:BJ:981:GLN:OE1 | 2:BJ:981:GLN:N | 2.29 | 0.63 |
| 3:CA:47:TRP:CZ3 | 3:CA:270:ARG:HD3 | 2.34 | 0.63 |
| 3:CB:292:ALA:HB1 | 3:CB:297:TYR:CE2 | 2.33 | 0.63 |
| 5:CH:318:GLN:HB3 | 6:CJ:4:LEU:HG | 1.81 | 0.63 |
| 6:CJ:16:ASP:OD2 | 6:CJ:45:LYS:NZ | 2.29 | 0.63 |
| 3:D:89:VAL:O | 3:D:246:THR:OG1 | 2.16 | 0.63 |
| 2:EC:872:SER:N | 2:EC:894:THR:HG21 | 2.11 | 0.63 |
| 5:EI:409:SER:N | 5:FA:444:ASN:O | 2.30 | 0.63 |
| 8:FI:43:ALA:CB | 8:IB:138:GLY:HA3 | 2.28 | 0.63 |
| 1:GE:492:TYR:HA | 1:GE:606:ILE:HD12 | 1.81 | 0.63 |
| 2:GF:1014:ASP:HA | 2:GF:1027:GLN:HB3 | 1.80 | 0.63 |
| 2:GF:326:VAL:HG21 | 2:GF:413:TRP:HZ2 | 1.63 | 0.63 |
| 2:GF:398:SER:OG | 2:GF:399:ALA:N | 2.31 | 0.63 |
| 3:GH:292:ALA:HB1 | 3:GH:297:TYR:HE2 | 1.62 | 0.63 |
| 5:HB:107:VAL:O | 5:HB:125:GLU:HG3 | 1.99 | 0.63 |
| 5:HC:318:GLN:NE2 | 6:HE:4:LEU:O | 2.31 | 0.63 |
| 5:HD:313:PHE:HE1 | 6:HF:8:ALA:HB1 | 1.62 | 0.63 |
| 7:HI:218:SER:O | 7:HI:227:VAL:HG22 | 1.98 | 0.63 |
| 5:I:102:TRP:CE3 | 5:I:131:SER:HB2 | 2.32 | 0.63 |
| 5:K:9:ASN:OD1 | 5:K:10:VAL:N | 2.30 | 0.63 |
| 7:P:167:GLN:NE2 | 6:HE:75:THR:HB | 2.14 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:193:LEU:HD21 | 7:Q:207:GLY:HA2 | 1.80 | 0.63 |
| 8:S:138:GLY:HA3 | 8:IB:43:ALA:CB | 2.28 | 0.63 |
| 12:W:167:GLU:HA | 12:IF:211:HIS:CE1 | 2.33 | 0.63 |
| 1:X:257:ILE:HG12 | 1:Y:331:ILE:HD11 | 1.81 | 0.63 |
| 1:X:98:TYR:HB2 | 1:X:332:LYS:HG2 | 1.80 | 0.63 |
| 1:X:90:VAL:O | 1:X:94:GLN:N | 2.26 | 0.63 |
| 1:Y:290:ASP:OD1 | 1:Y:291:THR:N | 2.28 | 0.63 |
| 13:YA:87[A]:LEU:HD21 | 13:YA:95[A]:ILE:HG23 | 1.80 | 0.63 |
| 13:YB:193[F]:ASP:OD1 | 13:YB:197[F]:TYR:N | 2.31 | 0.63 |
| 13:YB:442[A]:THR:HA | 13:YC:434[A]:THR:O | 1.99 | 0.63 |
| 13:YB:61[A]:ILE:HD11 | 13:YC:72[A]:SER:O | 1.98 | 0.63 |
| 13:YB:61[D]:ILE:HD11 | 13:YC:72[D]:SER:O | 1.98 | 0.63 |
| 14:YD:262[A]:SER:O | 14:YD:289[A]:ARG:NH1 | 2.32 | 0.63 |
| 14:YD:288[E]:TYR:OH | 14:YD:371[E]:LYS:NZ | 2.27 | 0.63 |
| 14:YD:312[A]:THR:OG1 | 14:YD:313[A]:ILE:N | 2.30 | 0.63 |
| 14:YE:262[B]:SER:O | 14:YE:289[B]:ARG:NH1 | 2.32 | 0.63 |
| 14:YF:262[C]:SER:O | 14:YF:289[C]:ARG:NH1 | 2.32 | 0.63 |
| 2:Z:180:ILE:HG13 | 2:Z:526:ILE:HD11 | 1.81 | 0.63 |
| 2:Z:312:THR:HG23 | 2:Z:370:SER:HB3 | 1.81 | 0.63 |
| 2:Z:326:VAL:HG21 | 2:Z:413:TRP:HZ2 | 1.64 | 0.63 |
| 2:Z:628:HIS:ND1 | 2:Z:628:HIS:O | 2.32 | 0.63 |
| 2:Z:98:GLU:OE1 | 2:Z:98:GLU:N | 2.30 | 0.63 |
| 1:A:510:MET:HB3 | 1:A:542:SER:HB3 | 1.79 | 0.63 |
| 1:A:98:TYR:HB2 | 1:A:332:LYS:HG2 | 1.80 | 0.63 |
| 4:AA:43:GLY:O | 4:AA:68:GLN:NE2 | 2.32 | 0.63 |
| 5:AC:13:ASP:OD1 | 5:AC:14:GLY:N | 2.32 | 0.63 |
| 5:AE:305:ASN:HB3 | 5:AE:388:ASN:HB2 | 1.79 | 0.63 |
| 5:AE:323:THR:HB | 5:AE:355:ASP:HB3 | 1.80 | 0.63 |
| 7:AI:418:ASP:OD1 | 7:AI:422:LYS:N | 2.30 | 0.63 |
| 7:AJ:212:PRO:HB2 | 7:BA:203:THR:HG22 | 1.81 | 0.63 |
| 1:B:148:ARG:HH22 | 1:B:196:GLN:HE22 | 1.46 | 0.63 |
| 1:BI:495:PRO:O | 1:BI:498:GLY:N | 2.32 | 0.63 |
| 1:BI:544:ASP:HB2 | 1:BI:576:ASP:HB2 | 1.80 | 0.63 |
| 2:BJ:180:ILE:HG13 | 2:BJ:526:ILE:HD11 | 1.81 | 0.63 |
| 2:BJ:584:GLY:HA3 | 2:BJ:597:TYR:OH | 1.98 | 0.63 |
| 2:C:121:LYS:HG2 | 2:C:158:VAL:HG22 | 1.80 | 0.63 |
| 2:C:186:ASP:OD1 | 2:C:187:ILE:N | 2.31 | 0.63 |
| 2:C:398:SER:OG | 2:C:399:ALA:N | 2.31 | 0.63 |
| 5:CG:318:GLN:NE2 | 6:CI:4:LEU:O | 2.32 | 0.63 |
| 5:CF:472:TYR:HA | 5:CG:416:ILE:HG23 | 1.80 | 0.63 |
| 3:E:135:ASP:OD1 | 3:E:136:VAL:N | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:1014:ASP:HA | 2:EC:1027:GLN:HB3 | 1.79 | 0.63 |
| 2:EC:821:ILE:C | 2:EC:824:GLN:HE22 | 2.01 | 0.63 |
| 2:EC:928:GLU:OE2 | 2:EC:960:GLY:HA2 | 1.98 | 0.63 |
| 3:ED:147:LEU:HD23 | 3:ED:149:ASP:H | 1.63 | 0.63 |
| 5:EI:30:PHE:HE1 | 5:FA:30:PHE:HE1 | 1.47 | 0.63 |
| 7:FE:476:ASP:O | 7:FE:479:ASN:ND2 | 2.31 | 0.63 |
| 7:FF:218:SER:O | 7:FF:227:VAL:HG22 | 1.98 | 0.63 |
| 2:GF:180:ILE:HG13 | 2:GF:526:ILE:HD11 | 1.81 | 0.63 |
| 5:HC:189:ASN:HD21 | 5:HD:150:GLN:NE2 | 1.96 | 0.63 |
| 7:O:194:ALA:HB2 | 7:O:208:TYR:HB3 | 1.81 | 0.63 |
| 1:X:424:TYR:HE2 | 1:X:655:LEU:HD13 | 1.63 | 0.63 |
| 13:YB:232[C]:ASN:CB | 13:YC:407[C]:PRO:HB3 | 2.28 | 0.63 |
| 13:YB:442[E]:THR:HA | 13:YC:434[E]:THR:O | 1.99 | 0.63 |
| 13:YB:575[E]:GLY:N | 13:YC:567[E]:ILE:O | 2.32 | 0.63 |
| 13:YB:61[E]:ILE:HD11 | 13:YC:72[E]:SER:O | 1.99 | 0.63 |
| 13:YA:47[E]:ILE:HG23 | 14:YD:123[E]:PRO:HG3 | 1.80 | 0.63 |
| 14:YD:17[C]:PHE:CE2 | 14:YD:28[C]:PHE:HB3 | 2.34 | 0.63 |
| 14:YD:305[A]:ASP:N | 14:YD:305[A]:ASP:OD1 | 2.31 | 0.63 |
| 14:YD:305[F]:ASP:N | 14:YD:305[F]:ASP:OD1 | 2.32 | 0.63 |
| 14:YF:17[A]:PHE:CE2 | 14:YF:28[A]:PHE:HB3 | 2.34 | 0.63 |
| 14:YF:188[A]:VAL:HG12 | 14:YF:197[A]:MET:HG2 | 1.81 | 0.63 |
| 14:YF:262[F]:SER:O | 14:YF:289[F]:ARG:NH1 | 2.32 | 0.63 |
| 14:YF:17[E]:PHE:CE2 | 14:YF:28[E]:PHE:HB3 | 2.34 | 0.63 |
| 14:YF:305[C]:ASP:N | 14:YF:305[C]:ASP:OD1 | 2.31 | 0.63 |
| 2:Z:81:ARG:HG2 | 2:Z:94:TRP:HE3 | 1.63 | 0.63 |
| 2:Z:928:GLU:OE2 | 2:Z:960:GLY:HA2 | 1.98 | 0.63 |
| 5:AC:248:MET:HB2 | 5:AC:254:TRP:NE1 | 2.13 | 0.63 |
| 5:AC:399:ILE:HG23 | 5:AE:399:ILE:HD13 | 1.80 | 0.63 |
| 7:AJ:218:SER:O | 7:AJ:227:VAL:HG22 | 1.98 | 0.63 |
| 8:BB:43:ALA:CB | 8:DE:138:GLY:HA3 | 2.28 | 0.63 |
| 8:BC:63:ASP:OD1 | 8:BC:64:ARG:N | 2.32 | 0.63 |
| 10:BE:222:ILE:HA | 10:BE:225:ILE:HG22 | 1.81 | 0.63 |
| 12:BG:211:HIS:CE1 | 12:DJ:167:GLU:HA | 2.34 | 0.63 |
| 1:BH:566:ASN:OD1 | 1:BH:567:GLU:N | 2.31 | 0.63 |
| 2:BJ:360:ASN:C | 2:BJ:362:LYS:H | 2.02 | 0.63 |
| 2:BJ:312:THR:HG23 | 2:BJ:370:SER:HB3 | 1.81 | 0.63 |
| 2:BJ:849:GLN:HG3 | 2:BJ:852:ILE:HD12 | 1.80 | 0.63 |
| 2:BJ:993:LEU:HD12 | 2:BJ:995:ASP:H | 1.63 | 0.63 |
| 2:C:584:GLY:HA3 | 2:C:597:TYR:OH | 1.98 | 0.63 |
| 4:CE:43:GLY:O | 4:CE:68:GLN:NE2 | 2.32 | 0.63 |
| 5:CF:111:ALA:HB2 | 5:CF:117:ILE:HG23 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:328:LEU:HD12 | 5:CH:330:HIS:HD2 | 1.64 | 0.63 |
| 5:CF:399:ILE:HG23 | 5:CH:399:ILE:HD13 | 1.80 | 0.63 |
| 5:CH:339:GLU:HB3 | 6:CI:172:SER:O | 1.99 | 0.63 |
| 7:DB:286:ASP:OD2 | 7:DD:291:ARG:NH1 | 2.32 | 0.63 |
| 7:DC:453:GLU:OE2 | 7:DC:471:THR:N | 2.31 | 0.63 |
| 1:EB:492:TYR:HA | 1:EB:606:ILE:HD12 | 1.81 | 0.63 |
| 2:EC:849:GLN:HG3 | 2:EC:852:ILE:HD12 | 1.80 | 0.63 |
| 2:EC:925:LEU:HD12 | 2:EC:993:LEU:HB3 | 1.80 | 0.63 |
| 4:EG:275:ALA:O | 4:EH:282:GLN:NE2 | 2.31 | 0.63 |
| 5:FA:196:ARG:NH1 | 7:FF:5:THR:O | 2.32 | 0.63 |
| 7:FF:214:THR:HA | 7:FF:217:ASN:ND2 | 2.13 | 0.63 |
| 7:FE:481:SER:OG | 7:FF:449:GLY:O | 2.09 | 0.63 |
| 8:DE:43:ALA:HB1 | 8:FH:138:GLY:HA3 | 1.79 | 0.63 |
| 8:FH:9:ALA:HB2 | 8:IA:34:PHE:HD2 | 1.64 | 0.63 |
| 10:GA:214:ARG:NH1 | 12:GC:246:ARG:HH12 | 1.95 | 0.63 |
| 1:GD:341:THR:HG21 | 2:GF:881:ARG:O | 1.98 | 0.63 |
| 1:GD:34:ILE:HG23 | 1:GD:48:PHE:HD2 | 1.62 | 0.63 |
| 3:E:233:GLN:HE22 | 2:GF:529:SER:H | 1.45 | 0.63 |
| 5:HC:391:GLY:HA3 | 5:HD:390:LEU:HD13 | 1.80 | 0.63 |
| 7:HH:230:LEU:HD23 | 7:HH:246:THR:HG22 | 1.81 | 0.63 |
| 7:HH:229:LYS:HG3 | 7:HH:243:VAL:HG12 | 1.81 | 0.63 |
| 2:C:921:TRP:NE1 | 5:J:19:LEU:HA | 2.13 | 0.63 |
| 5:J:318:GLN:NE2 | 6:L:4:LEU:O | 2.31 | 0.63 |
| 6:N:16:ASP:OD2 | 6:N:45:LYS:NZ | 2.29 | 0.63 |
| 7:O:211:SER:N | 7:O:214:THR:OG1 | 2.28 | 0.63 |
| 11:V:43:TYR:HE2 | 11:V:180:PHE:HB2 | 1.64 | 0.63 |
| 13:YB:30[A]:ARG:HB2 | 13:YB:52[A]:LEU:HD21 | 1.79 | 0.63 |
| 13:YB:563[F]:GLY:N | 13:YC:555[F]:ALA:O | 2.30 | 0.63 |
| 14:YD:17[E]:PHE:CE2 | 14:YD:28[E]:PHE:HB3 | 2.34 | 0.63 |
| 14:YD:60[D]:ILE:O | 14:YD:63[D]:LYS:N | 2.32 | 0.63 |
| 14:YE:17[A]:PHE:CE2 | 14:YE:28[A]:PHE:HB3 | 2.34 | 0.63 |
| 14:YE:17[C]:PHE:CE2 | 14:YE:28[C]:PHE:HB3 | 2.34 | 0.63 |
| 13:YC:572[B]:ILE:HD12 | 15:ZA:94[B]:VAL:HG22 | 1.80 | 0.63 |
| 1:A:90:VAL:O | 1:A:94:GLN:N | 2.26 | 0.63 |
| 5:AC:312:ARG:O | 5:AC:382:ASN:N | 2.24 | 0.63 |
| 5:AD:153:LYS:HG2 | 5:AD:154:ILE:H | 1.64 | 0.63 |
| 5:AE:318:GLN:HB3 | 6:AG:4:LEU:HG | 1.80 | 0.63 |
| 7:AI:310:ASN:OD1 | 7:AI:311:GLY:N | 2.32 | 0.63 |
| 7:AI:347:MET:HE3 | 7:AJ:347:MET:HB3 | 1.81 | 0.63 |
| 7:AJ:214:THR:HA | 7:AJ:217:ASN:ND2 | 2.13 | 0.63 |
| 11:BF:2:LEU:HD11 | 11:BF:71:TRP:CD2 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:358:GLN:HB2 | 1:BH:379:LYS:HB3 | 1.80 | 0.63 |
| 2:C:458:ASP:HB3 | 2:C:461:THR:OG1 | 1.99 | 0.63 |
| 2:C:957:PRO:O | 2:C:958:MET:HG2 | 1.99 | 0.63 |
| 3:CA:44:SER:O | 3:CA:270:ARG:NH1 | 2.31 | 0.63 |
| 5:CF:102:TRP:HE3 | 5:CF:131:SER:HB2 | 1.64 | 0.63 |
| 5:CF:13:ASP:OD1 | 5:CF:14:GLY:N | 2.32 | 0.63 |
| 5:CG:317:LEU:HD13 | 5:CH:312:ARG:HH22 | 1.62 | 0.63 |
| 5:CH:292:PRO:HA | 5:CH:368:ILE:HD12 | 1.80 | 0.63 |
| 8:DF:63:ASP:OD1 | 8:DF:64:ARG:N | 2.32 | 0.63 |
| 3:E:198:VAL:HG13 | 3:E:202:ARG:HG3 | 1.81 | 0.63 |
| 2:EC:398:SER:OG | 2:EC:399:ALA:N | 2.31 | 0.63 |
| 2:EC:423:GLU:N | 2:EC:423:GLU:OE1 | 2.30 | 0.63 |
| 1:EA:341:THR:HG21 | 2:EC:881:ARG:O | 1.98 | 0.63 |
| 2:EC:981:GLN:OE1 | 2:EC:981:GLN:N | 2.29 | 0.63 |
| 2:EC:33:TYR:HB3 | 3:ED:156:LEU:HD22 | 1.80 | 0.63 |
| 3:EE:292:ALA:HB1 | 3:EE:297:TYR:CE2 | 2.33 | 0.63 |
| 5:EI:13:ASP:OD1 | 5:EI:14:GLY:N | 2.32 | 0.63 |
| 5:EI:154:ILE:HG12 | 5:EJ:153:LYS:HZ2 | 1.62 | 0.63 |
| 5:EI:569:TYR:H | 5:EJ:550:VAL:HB | 1.63 | 0.63 |
| 5:EI:62:ALA:HB1 | 5:EI:82:PRO:HG3 | 1.80 | 0.63 |
| 7:FE:86:SER:HA | 7:FE:97:LEU:HD12 | 1.79 | 0.63 |
| 2:GF:168:ILE:HG23 | 2:GF:169:GLY:N | 2.14 | 0.63 |
| 2:GF:513:PHE:HB3 | 2:GF:525:TRP:CZ3 | 2.33 | 0.63 |
| 2:GF:52:ASN:OD1 | 2:GF:53:GLN:N | 2.27 | 0.63 |
| 3:GG:47:TRP:CZ3 | 3:GG:270:ARG:HD3 | 2.34 | 0.63 |
| 3:GH:135:ASP:OD1 | 3:GH:136:VAL:N | 2.31 | 0.63 |
| 7:HH:303:GLU:HA | 7:HI:309:ALA:HB3 | 1.80 | 0.63 |
| 7:HI:453:GLU:OE2 | 7:HI:471:THR:N | 2.31 | 0.63 |
| 5:I:13:ASP:OD1 | 5:I:14:GLY:N | 2.32 | 0.63 |
| 5:I:304:ILE:HG23 | 5:I:365:ILE:HD12 | 1.80 | 0.63 |
| 5:K:340:VAL:HG23 | 5:K:341:GLU:HG3 | 1.79 | 0.63 |
| 7:P:100:TYR:CE1 | 7:P:115:SER:HB2 | 2.34 | 0.63 |
| 8:S:79:HIS:HB2 | 8:IB:125:LYS:HG2 | 1.81 | 0.63 |
| 1:X:594:GLU:OE1 | 1:X:594:GLU:N | 2.32 | 0.63 |
| 1:Y:492:TYR:HA | 1:Y:606:ILE:HD12 | 1.81 | 0.63 |
| 13:YB:442[E]:THR:HG21 | 13:YC:438[E]:LEU:HD22 | 1.79 | 0.63 |
| 13:YB:61[B]:ILE:HG21 | 13:YC:59[B]:GLN:HA | 1.79 | 0.63 |
| 13:YA:61[E]:ILE:HD11 | 13:YB:72[E]:SER:O | 1.98 | 0.63 |
| 13:YA:533[B]:ASN:HD22 | 13:YC:540[B]:GLY:HA3 | 1.62 | 0.63 |
| 13:YB:575[C]:GLY:N | 13:YC:567[C]:ILE:O | 2.32 | 0.63 |
| 14:YD:188[E]:VAL:HG12 | 14:YD:197[E]:MET:HG2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:17[A]:PHE:CE2 | 14:YD:28[A]:PHE:HB3 | 2.34 | 0.63 |
| 14:YE:17[E]:PHE:CE2 | 14:YE:28[E]:PHE:HB3 | 2.34 | 0.63 |
| 14:YE:288[C]:TYR:OH | 14:YE:371[C]:LYS:NZ | 2.27 | 0.63 |
| 14:YE:305[D]:ASP:OD1 | 14:YE:305[D]:ASP:N | 2.32 | 0.63 |
| 14:YF:17[C]:PHE:CE2 | 14:YF:28[C]:PHE:HB3 | 2.34 | 0.63 |
| 13:YC:24[E]:LEU:HD23 | 14:YF:259[E]:LEU:HD22 | 1.81 | 0.63 |
| 2:Z:752:TYR:OH | 2:Z:878:ASP:OD2 | 2.11 | 0.63 |
| 5:AC:365:ILE:HB | 5:AC:366:PRO:CD | 2.29 | 0.63 |
| 5:AD:65:GLY:O | 5:AE:45:SER:OG | 2.13 | 0.63 |
| 5:AE:328:LEU:HD12 | 5:AE:330:HIS:HD2 | 1.64 | 0.63 |
| 7:BA:310:ASN:OD1 | 7:BA:311:GLY:N | 2.31 | 0.63 |
| 11:BF:43:TYR:HE2 | 11:BF:180:PHE:HB2 | 1.64 | 0.63 |
| 2:C:168:ILE:HG23 | 2:C:169:GLY:N | 2.14 | 0.63 |
| 2:C:993:LEU:HD12 | 2:C:995:ASP:H | 1.63 | 0.63 |
| 3:CA:89:VAL:O | 3:CA:246:THR:OG1 | 2.16 | 0.63 |
| 5:CF:248:MET:HB2 | 5:CF:254:TRP:NE1 | 2.13 | 0.63 |
| 6:CJ:17:PHE:O | 6:DA:13:ARG:NH1 | 2.23 | 0.63 |
| 3:D:270:ARG:CZ | 3:D:317:PRO:HB3 | 2.28 | 0.63 |
| 3:D:44:SER:O | 3:D:270:ARG:NH1 | 2.31 | 0.63 |
| 7:DC:212:PRO:HB2 | 7:DD:203:THR:HG22 | 1.81 | 0.63 |
| 7:DD:476:ASP:OD1 | 7:DD:479:ASN:ND2 | 2.30 | 0.63 |
| 2:EC:168:ILE:HG23 | 2:EC:169:GLY:N | 2.14 | 0.63 |
| 2:EC:312:THR:HG23 | 2:EC:370:SER:HB3 | 1.81 | 0.63 |
| 2:EC:788:THR:HG23 | 2:EC:790:THR:H | 1.63 | 0.63 |
| 3:ED:47:TRP:CZ3 | 3:ED:270:ARG:HD3 | 2.34 | 0.63 |
| 5:EJ:317:LEU:HD13 | 5:FA:312:ARG:HH22 | 1.61 | 0.63 |
| 5:EI:459:ILE:HD11 | 5:FA:463:ALA:HB2 | 1.81 | 0.63 |
| 7:FE:230:LEU:HD23 | 7:FE:246:THR:HG22 | 1.81 | 0.63 |
| 7:FE:513:ARG:O | 7:FF:441:GLN:N | 2.28 | 0.63 |
| 7:FF:100:TYR:CE1 | 7:FF:115:SER:HB2 | 2.34 | 0.63 |
| 11:GB:43:TYR:HE2 | 11:GB:180:PHE:HB2 | 1.64 | 0.63 |
| 12:GC:211:HIS:CE1 | 12:IF:167:GLU:HA | 2.33 | 0.63 |
| 1:GD:242:GLU:O | 1:GD:256:TYR:OH | 2.16 | 0.63 |
| 1:GD:594:GLU:N | 1:GD:594:GLU:OE1 | 2.32 | 0.63 |
| 1:GE:386:THR:OG1 | 1:GE:390:GLU:OE2 | 2.17 | 0.63 |
| 2:GF:1012:LEU:HD13 | 2:GF:1027:GLN:CD | 2.18 | 0.63 |
| 2:GF:458:ASP:HB3 | 2:GF:461:THR:OG1 | 1.99 | 0.63 |
| 2:GF:788:THR:HG23 | 2:GF:790:THR:H | 1.63 | 0.63 |
| 5:HC:327:PRO:HG3 | 5:HD:264:ARG:HD3 | 1.81 | 0.63 |
| 5:HD:9:ASN:OD1 | 5:HD:10:VAL:N | 2.30 | 0.63 |
| 8:IB:63:ASP:OD1 | 8:IB:64:ARG:N | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:507:ASP:OD1 | 5:J:511:ASN:N | 2.22 | 0.63 |
| 7:Q:4:ASN:OD1 | 7:Q:15:TYR:OH | 2.17 | 0.63 |
| 1:Y:544:ASP:HB2 | 1:Y:576:ASP:HB2 | 1.80 | 0.63 |
| 13:YB:95[E]:ILE:HD11 | 13:YC:83[E]:TYR:CZ | 2.34 | 0.63 |
| 14:YD:125[D]:PHE:CE2 | 14:YD:134[D]:GLU:HG3 | 2.30 | 0.63 |
| 14:YD:305[E]:ASP:OD1 | 14:YD:305[E]:ASP:N | 2.32 | 0.63 |
| 14:YE:188[C]:VAL:HG12 | 14:YE:197[C]:MET:HG2 | 1.81 | 0.63 |
| 14:YE:305[B]:ASP:OD1 | 14:YE:305[B]:ASP:N | 2.31 | 0.63 |
| 14:YE:60[B]:ILE:O | 14:YE:63[B]:LYS:N | 2.32 | 0.63 |
| 14:YF:188[B]:VAL:HG12 | 14:YF:197[B]:MET:HG2 | 1.81 | 0.63 |
| 13:YC:24[F]:LEU:HD23 | 14:YF:259[F]:LEU:HD22 | 1.81 | 0.63 |
| 14:YF:66[F]:GLY:N | 14:YF:68[F]:GLU:OE2 | 2.32 | 0.63 |
| 1:A:341:THR:HG21 | 2:C:881:ARG:O | 1.99 | 0.62 |
| 6:AG:52:ILE:HD11 | 6:AH:15:ALA:HB2 | 1.81 | 0.62 |
| 1:A:337:GLN:HG3 | 1:B:334:GLU:HG2 | 1.79 | 0.62 |
| 8:BB:63:ASP:OD1 | 8:BB:64:ARG:N | 2.32 | 0.62 |
| 1:BH:424:TYR:HE2 | 1:BH:655:LEU:HD13 | 1.63 | 0.62 |
| 1:BI:492:TYR:HA | 1:BI:606:ILE:HD12 | 1.81 | 0.62 |
| 2:BJ:121:LYS:HG2 | 2:BJ:158:VAL:HG22 | 1.80 | 0.62 |
| 2:BJ:81:ARG:HG2 | 2:BJ:94:TRP:HE3 | 1.63 | 0.62 |
| 2:BJ:957:PRO:O | 2:BJ:958:MET:HG2 | 1.99 | 0.62 |
| 3:CA:270:ARG:CZ | 3:CA:317:PRO:HB3 | 2.28 | 0.62 |
| 4:CE:106:CYS:SG | 4:CE:149:ARG:NH2 | 2.67 | 0.62 |
| 5:CG:371:PHE:CZ | 5:CG:373:SER:HB3 | 2.34 | 0.62 |
| 7:DC:218:SER:O | 7:DC:227:VAL:HG22 | 1.98 | 0.62 |
| 8:DE:63:ASP:OD1 | 8:DE:64:ARG:N | 2.32 | 0.62 |
| 1:EA:358:GLN:HB2 | 1:EA:379:LYS:HB3 | 1.80 | 0.62 |
| 2:EC:957:PRO:O | 2:EC:958:MET:HG2 | 1.99 | 0.62 |
| 5:EI:102:TRP:HE3 | 5:EI:131:SER:HB2 | 1.64 | 0.62 |
| 5:EI:248:MET:HB2 | 5:EI:254:TRP:NE1 | 2.13 | 0.62 |
| 5:EJ:212:PHE:HZ | 5:EJ:230:ILE:HB | 1.63 | 0.62 |
| 5:FA:328:LEU:HD12 | 5:FA:330:HIS:HD2 | 1.64 | 0.62 |
| 7:FG:476:ASP:OD1 | 7:FG:479:ASN:ND2 | 2.30 | 0.62 |
| 8:FH:63:ASP:OD1 | 8:FH:64:ARG:N | 2.32 | 0.62 |
| 8:FI:125:LYS:HG2 | 8:IB:79:HIS:HB2 | 1.82 | 0.62 |
| 11:GB:135:ASP:CG | 11:GB:136:LYS:H | 2.03 | 0.62 |
| 1:GD:517:PHE:N | 1:GD:536:TYR:O | 2.24 | 0.62 |
| 1:GD:543:THR:HG21 | 1:GD:552:LYS:H | 1.62 | 0.62 |
| 3:GG:44:SER:O | 3:GG:270:ARG:NH1 | 2.31 | 0.62 |
| 4:GJ:106:CYS:SG | 4:GJ:149:ARG:NH2 | 2.67 | 0.62 |
| 5:HB:237:ASN:OD1 | 5:HB:238:ILE:N | 2.31 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:476:ASP:O | 7:HH:479:ASN:ND2 | 2.31 | 0.62 |
| 7:HI:100:TYR:CE1 | 7:HI:115:SER:HB2 | 2.34 | 0.62 |
| 8:IA:63:ASP:OD1 | 8:IA:64:ARG:N | 2.32 | 0.62 |
| 11:IE:135:ASP:CG | 11:IE:136:LYS:H | 2.03 | 0.62 |
| 1:GD:84:ASN:ND2 | 11:IE:14:LYS:O | 2.31 | 0.62 |
| 11:IE:2:LEU:HD11 | 11:IE:71:TRP:CD2 | 2.33 | 0.62 |
| 5:K:119:GLY:H | 5:K:142:ARG:HH22 | 1.46 | 0.62 |
| 5:K:330:HIS:ND1 | 5:K:355:ASP:HB2 | 2.14 | 0.62 |
| 7:P:214:THR:HA | 7:P:217:ASN:ND2 | 2.14 | 0.62 |
| 13:YB:575[F]:GLY:N | 13:YC:567[F]:ILE:O | 2.32 | 0.62 |
| 13:YB:61[F]:ILE:HG12 | 13:YC:60[F]:PRO:CD | 2.29 | 0.62 |
| 14:YD:245[C]:ARG:NE | 14:YD:246[C]:ASP:OD1 | 2.25 | 0.62 |
| 14:YD:305[B]:ASP:OD1 | 14:YD:305[B]:ASP:N | 2.31 | 0.62 |
| 14:YE:215[C]:GLU:OE1 | 14:YF:100[C]:LYS:NZ | 2.32 | 0.62 |
| 14:YE:262[A]:SER:O | 14:YE:289[A]:ARG:NH1 | 2.32 | 0.62 |
| 14:YE:312[A]:THR:OG1 | 14:YE:313[A]:ILE:N | 2.30 | 0.62 |
| 14:YF:262[E]:SER:O | 14:YF:289[E]:ARG:NH1 | 2.32 | 0.62 |
| 2:Z:1012:LEU:HD13 | 2:Z:1027:GLN:CD | 2.18 | 0.62 |
| 2:Z:513:PHE:HB3 | 2:Z:525:TRP:CZ3 | 2.33 | 0.62 |
| 1:A:594:GLU:OE1 | 1:A:594:GLU:N | 2.32 | 0.62 |
| 5:AC:102:TRP:HE3 | 5:AC:131:SER:HB2 | 1.64 | 0.62 |
| 5:AD:320:LEU:HG | 5:AD:357:SER:HB3 | 1.80 | 0.62 |
| 5:AD:147:LYS:HB2 | 5:AE:153:LYS:HB2 | 1.81 | 0.62 |
| 5:AE:195:HIS:N | 5:AE:197:GLY:O | 2.31 | 0.62 |
| 5:AE:313:PHE:HE1 | 6:AG:8:ALA:HB1 | 1.63 | 0.62 |
| 1:B:521:ARG:O | 1:B:533:ASP:HB2 | 1.97 | 0.62 |
| 1:BH:594:GLU:OE1 | 1:BH:594:GLU:N | 2.32 | 0.62 |
| 1:BI:155:ARG:HA | 1:BI:161:TYR:HB3 | 1.81 | 0.62 |
| 1:BI:148:ARG:HH22 | 1:BI:196:GLN:HE22 | 1.46 | 0.62 |
| 2:BJ:168:ILE:HG23 | 2:BJ:169:GLY:N | 2.14 | 0.62 |
| 2:BJ:950:GLU:N | 2:BJ:950:GLU:OE1 | 2.24 | 0.62 |
| 2:C:1012:LEU:HD13 | 2:C:1027:GLN:CD | 2.18 | 0.62 |
| 2:C:92:SER:OG | 2:C:93:ASP:N | 2.32 | 0.62 |
| 2:C:940:GLY:O | 5:I:21:LYS:NZ | 2.31 | 0.62 |
| 5:CF:304:ILE:HG23 | 5:CF:365:ILE:HD12 | 1.80 | 0.62 |
| 5:CF:387:ASN:HB3 | 5:CF:389:ASP:OD1 | 1.98 | 0.62 |
| 5:CG:147:LYS:HB2 | 5:CH:153:LYS:HB2 | 1.81 | 0.62 |
| 5:CG:159:ILE:HG22 | 5:CG:161:ASN:O | 1.99 | 0.62 |
| 5:CG:198:ASN:HD22 | 5:CH:194:LYS:HD3 | 1.64 | 0.62 |
| 7:DD:27:PRO:HA | 7:DD:29:ILE:HD11 | 1.82 | 0.62 |
| 12:DJ:216:PHE:HE1 | 12:DJ:218:MET:HE3 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:117:GLN:O | 2:EC:596:SER:OG | 2.15 | 0.62 |
| 2:EC:513:PHE:HB3 | 2:EC:525:TRP:CZ3 | 2.33 | 0.62 |
| 2:EC:52:ASN:OD1 | 2:EC:53:GLN:N | 2.27 | 0.62 |
| 5:EI:206:PHE:HZ | 5:EI:221:GLU:HG2 | 1.63 | 0.62 |
| 5:EI:387:ASN:HB3 | 5:EI:389:ASP:OD1 | 1.98 | 0.62 |
| 5:EJ:320:LEU:HG | 5:EJ:357:SER:HB3 | 1.80 | 0.62 |
| 7:FE:194:ALA:HB2 | 7:FE:208:TYR:HB3 | 1.81 | 0.62 |
| 7:FE:77:THR:HG21 | 7:FF:72:ASN:HA | 1.82 | 0.62 |
| 7:FG:64:GLN:O | 7:FG:68:ASP:N | 2.27 | 0.62 |
| 2:GF:33:TYR:HB3 | 3:GG:156:LEU:HD22 | 1.80 | 0.62 |
| 2:GF:436:THR:HG22 | 2:GF:441:VAL:HG12 | 1.79 | 0.62 |
| 1:GD:60:LEU:HD22 | 2:GF:671:TYR:CE1 | 2.35 | 0.62 |
| 2:GF:993:LEU:HD12 | 2:GF:995:ASP:H | 1.63 | 0.62 |
| 3:GG:292:ALA:HB1 | 3:GG:297:TYR:CE2 | 2.35 | 0.62 |
| 5:I:234:GLN:NE2 | 7:Q:9:VAL:HG21 | 2.14 | 0.62 |
| 5:I:263:ILE:HG22 | 5:I:381:ILE:HB | 1.79 | 0.62 |
| 5:J:153:LYS:HG2 | 5:J:154:ILE:H | 1.64 | 0.62 |
| 5:J:371:PHE:CZ | 5:J:373:SER:HB3 | 2.34 | 0.62 |
| 5:K:323:THR:HB | 5:K:355:ASP:HB3 | 1.80 | 0.62 |
| 5:K:318:GLN:HB3 | 6:M:4:LEU:HG | 1.82 | 0.62 |
| 10:U:222:ILE:HA | 10:U:225:ILE:HG22 | 1.81 | 0.62 |
| 12:W:216:PHE:CE1 | 12:W:218:MET:HE3 | 2.34 | 0.62 |
| 1:X:566:ASN:OD1 | 1:X:567:GLU:N | 2.31 | 0.62 |
| 1:Y:87:SER:OG | 1:Y:230:ILE:O | 2.11 | 0.62 |
| 13:YB:442[D]:THR:HG21 | 13:YC:438[D]:LEU:HD22 | 1.79 | 0.62 |
| 14:YD:188[F]:VAL:HG12 | 14:YD:197[F]:MET:HG2 | 1.81 | 0.62 |
| 14:YD:262[C]:SER:O | 14:YD:289[C]:ARG:NH1 | 2.32 | 0.62 |
| 14:YE:188[B]:VAL:HG12 | 14:YE:197[B]:MET:HG2 | 1.81 | 0.62 |
| 14:YE:188[D]:VAL:HG12 | 14:YE:197[D]:MET:HG2 | 1.81 | 0.62 |
| 14:YE:245[A]:ARG:NE | 14:YE:246[A]:ASP:OD1 | 2.25 | 0.62 |
| 14:YE:262[D]:SER:O | 14:YE:289[D]:ARG:NH1 | 2.32 | 0.62 |
| 14:YE:305[E]:ASP:OD1 | 14:YE:305[E]:ASP:N | 2.32 | 0.62 |
| 14:YE:66[B]:GLY:N | 14:YE:68[B]:GLU:OE2 | 2.33 | 0.62 |
| 10:ID:285:LEU:HA | 14:YF:215[B]:GLU:CG | 2.29 | 0.62 |
| 14:YF:262[B]:SER:O | 14:YF:289[B]:ARG:NH1 | 2.32 | 0.62 |
| 14:YE:332[F]:GLN:HB3 | 14:YF:61[F]:HIS:CE1 | 2.34 | 0.62 |
| 2:Z:360:ASN:C | 2:Z:362:LYS:H | 2.02 | 0.62 |
| 5:AC:38:GLY:HA2 | 5:AC:43:PRO:HA | 1.80 | 0.62 |
| 5:AD:212:PHE:CZ | 5:AD:230:ILE:HB | 2.34 | 0.62 |
| 5:AE:119:GLY:H | 5:AE:142:ARG:HH22 | 1.46 | 0.62 |
| 5:AC:251:VAL:HG11 | 5:AE:254:TRP:CZ2 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AF:60:HIS:NE2 | 6:AH:28:ASP:OD2 | 2.30 | 0.62 |
| 1:BH:96:ASN:HB3 | 1:BH:333:ARG:HB2 | 1.82 | 0.62 |
| 2:BJ:458:ASP:HB3 | 2:BJ:461:THR:OG1 | 1.99 | 0.62 |
| 3:CB:198:VAL:HG13 | 3:CB:202:ARG:HG3 | 1.81 | 0.62 |
| 5:CH:214:SER:OG | 5:CH:222:LEU:O | 2.16 | 0.62 |
| 7:DC:100:TYR:CE1 | 7:DC:115:SER:HB2 | 2.34 | 0.62 |
| 3:E:42:GLY:HA2 | 3:E:76:MET:HG2 | 1.79 | 0.62 |
| 1:EA:543:THR:HG21 | 1:EA:552:LYS:H | 1.62 | 0.62 |
| 3:EE:135:ASP:OD1 | 3:EE:136:VAL:N | 2.31 | 0.62 |
| 5:EJ:103:ASN:N | 5:EJ:127:ASN:O | 2.31 | 0.62 |
| 5:EJ:212:PHE:CZ | 5:EJ:230:ILE:HB | 2.34 | 0.62 |
| 7:FE:160:MET:SD | 7:FG:165:THR:HG21 | 2.39 | 0.62 |
| 8:DE:43:ALA:CB | 8:FH:138:GLY:HA3 | 2.29 | 0.62 |
| 2:GF:81:ARG:HG2 | 2:GF:94:TRP:HE3 | 1.63 | 0.62 |
| 2:GF:957:PRO:O | 2:GF:958:MET:HG2 | 1.99 | 0.62 |
| 3:GH:294:LYS:N | 3:GH:297:TYR:OH | 2.32 | 0.62 |
| 5:HC:212:PHE:CZ | 5:HC:230:ILE:HB | 2.34 | 0.62 |
| 5:I:62:ALA:HB1 | 5:I:82:PRO:HG3 | 1.80 | 0.62 |
| 10:ID:206:VAL:HG22 | 10:ID:347:THR:HG22 | 1.82 | 0.62 |
| 8:S:63:ASP:OD1 | 8:S:64:ARG:N | 2.32 | 0.62 |
| 13:YB:538[C]:VAL:HG11 | 13:YC:534[C]:LEU:HB2 | 1.79 | 0.62 |
| 14:YD:188[D]:VAL:HG12 | 14:YD:197[D]:MET:HG2 | 1.81 | 0.62 |
| 14:YD:215[A]:GLU:OE1 | 14:YE:100[A]:LYS:NZ | 2.33 | 0.62 |
| 14:YD:262[E]:SER:O | 14:YD:289[E]:ARG:NH1 | 2.32 | 0.62 |
| 14:YD:262[F]:SER:O | 14:YD:289[F]:ARG:NH1 | 2.32 | 0.62 |
| 14:YD:262[B]:SER:O | 14:YD:289[B]:ARG:NH1 | 2.32 | 0.62 |
| 14:YD:60[C]:ILE:O | 14:YD:63[C]:LYS:N | 2.32 | 0.62 |
| 14:YD:60[E]:ILE:O | 14:YD:63[E]:LYS:N | 2.32 | 0.62 |
| 14:YE:125[B]:PHE:CE2 | 14:YE:134[B]:GLU:HG3 | 2.30 | 0.62 |
| 14:YE:17[B]:PHE:CE2 | 14:YE:28[B]:PHE:HB3 | 2.35 | 0.62 |
| 14:YE:262[C]:SER:O | 14:YE:289[C]:ARG:NH1 | 2.32 | 0.62 |
| 14:YE:305[F]:ASP:OD1 | 14:YE:305[F]:ASP:N | 2.32 | 0.62 |
| 14:YE:60[C]:ILE:O | 14:YE:63[C]:LYS:N | 2.32 | 0.62 |
| 14:YF:125[F]:PHE:CE2 | 14:YF:134[F]:GLU:HG3 | 2.30 | 0.62 |
| 14:YF:245[E]:ARG:NE | 14:YF:246[E]:ASP:OD1 | 2.25 | 0.62 |
| 14:YF:262[D]:SER:O | 14:YF:289[D]:ARG:NH1 | 2.32 | 0.62 |
| 2:Z:75:LEU:HA | 2:Z:103:PHE:HA | 1.82 | 0.62 |
| 2:Z:925:LEU:HD12 | 2:Z:993:LEU:HB3 | 1.80 | 0.62 |
| 5:AD:172:GLN:HG2 | 5:AD:173:GLY:H | 1.65 | 0.62 |
| 5:AE:292:PRO:HA | 5:AE:368:ILE:HD12 | 1.80 | 0.62 |
| 5:AE:196:ARG:NH1 | 7:AJ:8:HIS:HB3 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:290:ASP:OD1 | 1:B:291:THR:N | 2.28 | 0.62 |
| 7:BA:120:LYS:O | 7:BA:124:ALA:N | 2.32 | 0.62 |
| 7:BA:162:PRO:HA | 7:BA:165:THR:HG22 | 1.82 | 0.62 |
| 7:BA:66:VAL:HG21 | 7:BA:80:THR:HB | 1.82 | 0.62 |
| 8:BB:56:ARG:NH2 | 8:FH:96:GLY:O | 2.33 | 0.62 |
| 10:BE:206:VAL:HG22 | 10:BE:347:THR:HG22 | 1.82 | 0.62 |
| 2:BJ:117:GLN:O | 2:BJ:596:SER:OG | 2.15 | 0.62 |
| 2:BJ:628:HIS:O | 2:BJ:628:HIS:ND1 | 2.32 | 0.62 |
| 7:DB:310:ASN:OD1 | 7:DB:311:GLY:N | 2.32 | 0.62 |
| 1:EA:594:GLU:OE1 | 1:EA:594:GLU:N | 2.32 | 0.62 |
| 2:EC:458:ASP:HB3 | 2:EC:461:THR:OG1 | 1.99 | 0.62 |
| 2:EC:514:PHE:HB3 | 2:EC:523:ARG:HB3 | 1.82 | 0.62 |
| 5:EJ:159:ILE:HG22 | 5:EJ:161:ASN:O | 1.99 | 0.62 |
| 5:FA:292:PRO:HA | 5:FA:368:ILE:HD12 | 1.80 | 0.62 |
| 5:FA:313:PHE:HB3 | 5:FA:381:ILE:HG12 | 1.81 | 0.62 |
| 8:FH:56:ARG:HD3 | 8:IA:64:ARG:HD3 | 1.81 | 0.62 |
| 11:GB:112:HIS:HB3 | 11:GB:150:LEU:HD13 | 1.81 | 0.62 |
| 1:GE:148:ARG:HH22 | 1:GE:196:GLN:HE22 | 1.46 | 0.62 |
| 2:GF:121:LYS:HG2 | 2:GF:158:VAL:HG22 | 1.80 | 0.62 |
| 5:HB:102:TRP:HE3 | 5:HB:131:SER:HB2 | 1.64 | 0.62 |
| 5:HD:313:PHE:HB3 | 5:HD:381:ILE:HG12 | 1.81 | 0.62 |
| 5:HD:318:GLN:HB3 | 6:HF:4:LEU:HG | 1.81 | 0.62 |
| 5:HD:323:THR:HB | 5:HD:355:ASP:HB3 | 1.81 | 0.62 |
| 5:HC:542:LEU:HD11 | 5:HD:569:TYR:CE2 | 2.35 | 0.62 |
| 7:HI:146:SER:HA | 7:HI:164:LYS:NZ | 2.14 | 0.62 |
| 6:FB:75:THR:HB | 7:HI:167:GLN:NE2 | 2.15 | 0.62 |
| 5:I:107:VAL:O | 5:I:125:GLU:HG3 | 1.98 | 0.62 |
| 8:IA:43:ALA:O | 8:IA:162:TRP:NE1 | 2.33 | 0.62 |
| 5:I:264:ARG:HB3 | 5:K:326:MET:CE | 2.28 | 0.62 |
| 5:K:313:PHE:HB3 | 5:K:381:ILE:HG12 | 1.81 | 0.62 |
| 5:K:339:GLU:HB3 | 6:L:172:SER:O | 1.99 | 0.62 |
| 7:O:140:GLY:HA2 | 7:Q:129:PHE:CZ | 2.34 | 0.62 |
| 1:X:242:GLU:O | 1:X:256:TYR:OH | 2.16 | 0.62 |
| 1:Y:386:THR:OG1 | 1:Y:390:GLU:OE2 | 2.17 | 0.62 |
| 13:YB:304[F]:TRP:O | 13:YB:308[F]:TYR:N | 2.33 | 0.62 |
| 13:YB:232[F]:ASN:CB | 13:YC:407[F]:PRO:HB3 | 2.28 | 0.62 |
| 14:YD:100[E]:LYS:NZ | 14:YF:215[E]:GLU:OE1 | 2.32 | 0.62 |
| 14:YD:127[A]:ASP:OD1 | 14:YD:129[A]:GLY:N | 2.33 | 0.62 |
| 14:YD:127[B]:ASP:OD1 | 14:YD:129[B]:GLY:N | 2.33 | 0.62 |
| 14:YD:305[D]:ASP:OD1 | 14:YD:305[D]:ASP:N | 2.32 | 0.62 |
| 14:YD:66[D]:GLY:N | 14:YD:68[D]:GLU:OE2 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:188[A]:VAL:HG12 | 14:YE:197[A]:MET:HG2 | 1.81 | 0.62 |
| 14:YE:60[D]:ILE:O | 14:YE:63[D]:LYS:N | 2.32 | 0.62 |
| 14:YF:127[B]:ASP:OD1 | 14:YF:129[B]:GLY:N | 2.33 | 0.62 |
| 14:YF:305[D]:ASP:OD1 | 14:YF:305[D]:ASP:N | 2.32 | 0.62 |
| 14:YF:305[F]:ASP:N | 14:YF:305[F]:ASP:OD1 | 2.32 | 0.62 |
| 14:YF:60[E]:ILE:O | 14:YF:63[E]:LYS:N | 2.32 | 0.62 |
| 1:A:34:ILE:HG23 | 1:A:48:PHE:HD2 | 1.62 | 0.62 |
| 5:AC:107:VAL:O | 5:AC:125:GLU:HG3 | 1.99 | 0.62 |
| 5:AC:36:GLU:HA | 5:AC:50:LYS:HZ1 | 1.63 | 0.62 |
| 5:AC:71:ASN:OD1 | 5:AC:73:SER:N | 2.27 | 0.62 |
| 5:AD:159:ILE:HG22 | 5:AD:161:ASN:O | 1.99 | 0.62 |
| 7:AJ:146:SER:HA | 7:AJ:164:LYS:NZ | 2.14 | 0.62 |
| 7:AI:77:THR:HG21 | 7:AJ:72:ASN:HA | 1.81 | 0.62 |
| 1:B:155:ARG:HA | 1:B:161:TYR:HB3 | 1.81 | 0.62 |
| 9:BD:19:TRP:CE3 | 9:BD:20:ASN:HB3 | 2.35 | 0.62 |
| 3:CB:135:ASP:OD1 | 3:CB:136:VAL:N | 2.31 | 0.62 |
| 5:CG:196:ARG:HE | 7:DD:5:THR:HG23 | 1.64 | 0.62 |
| 5:CG:320:LEU:HG | 5:CG:357:SER:HB3 | 1.80 | 0.62 |
| 7:DB:77:THR:HG21 | 7:DC:72:ASN:HA | 1.81 | 0.62 |
| 10:DH:132:SER:HA | 10:DH:209:TRP:HE1 | 1.64 | 0.62 |
| 2:EC:897:THR:HG22 | 3:EE:329:ASN:HB2 | 1.80 | 0.62 |
| 3:ED:89:VAL:O | 3:ED:246:THR:OG1 | 2.16 | 0.62 |
| 3:ED:292:ALA:HB1 | 3:ED:297:TYR:CE2 | 2.35 | 0.62 |
| 5:EJ:153:LYS:HG2 | 5:EJ:154:ILE:H | 1.64 | 0.62 |
| 8:FH:125:LYS:HG2 | 8:IA:79:HIS:HB2 | 1.82 | 0.62 |
| 1:GE:543:THR:OG1 | 1:GE:544:ASP:N | 2.29 | 0.62 |
| 2:GF:415:ARG:HH12 | 2:GF:424:ARG:HH22 | 1.48 | 0.62 |
| 2:GF:514:PHE:HB3 | 2:GF:523:ARG:HB3 | 1.82 | 0.62 |
| 2:GF:928:GLU:OE2 | 2:GF:960:GLY:HA2 | 1.98 | 0.62 |
| 2:GF:925:LEU:HD12 | 2:GF:993:LEU:HB3 | 1.80 | 0.62 |
| 3:GG:89:VAL:O | 3:GG:246:THR:OG1 | 2.16 | 0.62 |
| 3:GH:219:ASP:OD1 | 3:GH:221:THR:N | 2.32 | 0.62 |
| 5:HB:111:ALA:HB2 | 5:HB:117:ILE:HG23 | 1.80 | 0.62 |
| 5:HC:371:PHE:CZ | 5:HC:373:SER:HB3 | 2.34 | 0.62 |
| 6:HE:11:ILE:HA | 6:HG:7:LYS:HD3 | 1.82 | 0.62 |
| 7:HH:347:MET:HE3 | 7:HI:347:MET:HB3 | 1.81 | 0.62 |
| 5:I:111:ALA:HB2 | 5:I:117:ILE:HG23 | 1.80 | 0.62 |
| 5:I:102:TRP:HE3 | 5:I:131:SER:HB2 | 1.64 | 0.62 |
| 5:I:30:PHE:HE1 | 5:K:30:PHE:HE1 | 1.47 | 0.62 |
| 9:IC:19:TRP:CE3 | 9:IC:20:ASN:HB3 | 2.35 | 0.62 |
| 5:J:147:LYS:HB2 | 5:K:153:LYS:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:172:GLN:HG2 | 5:J:173:GLY:H | 1.64 | 0.62 |
| 7:O:309:ALA:HB3 | 7:Q:303:GLU:HA | 1.82 | 0.62 |
| 8:S:43:ALA:O | 8:S:162:TRP:NE1 | 2.33 | 0.62 |
| 10:U:206:VAL:HG22 | 10:U:347:THR:HG22 | 1.82 | 0.62 |
| 11:V:112:HIS:HB3 | 11:V:150:LEU:HD13 | 1.81 | 0.62 |
| 11:V:135:ASP:CG | 11:V:136:LYS:H | 2.03 | 0.62 |
| 1:X:96:ASN:HB3 | 1:X:333:ARG:HB2 | 1.82 | 0.62 |
| 13:YB:193[D]:ASP:OD1 | 13:YB:197[D]:TYR:N | 2.33 | 0.62 |
| 13:YB:304[C]:TRP:O | 13:YB:308[C]:TYR:N | 2.33 | 0.62 |
| 13:YB:50[A]:GLU:N | 13:YB:50[A]:GLU:OE2 | 2.33 | 0.62 |
| 13:YB:7[E]:ASN:ND2 | 13:YC:9[E]:ASN:HA | 2.14 | 0.62 |
| 14:YD:127[F]:ASP:OD1 | 14:YD:129[F]:GLY:N | 2.33 | 0.62 |
| 11:GB:178:ASN:N | 14:YD:217[E]:SER:O | 2.31 | 0.62 |
| 14:YD:61[A]:HIS:CE1 | 14:YF:332[A]:GLN:HB3 | 2.34 | 0.62 |
| 14:YE:127[F]:ASP:OD1 | 14:YE:129[F]:GLY:N | 2.33 | 0.62 |
| 14:YE:127[D]:ASP:OD1 | 14:YE:129[D]:GLY:N | 2.33 | 0.62 |
| 14:YE:262[F]:SER:O | 14:YE:289[F]:ARG:NH1 | 2.32 | 0.62 |
| 14:YF:127[C]:ASP:OD1 | 14:YF:129[C]:GLY:N | 2.33 | 0.62 |
| 14:YF:127[D]:ASP:OD1 | 14:YF:129[D]:GLY:N | 2.33 | 0.62 |
| 14:YF:17[B]:PHE:CE2 | 14:YF:28[B]:PHE:HB3 | 2.35 | 0.62 |
| 14:YF:188[E]:VAL:HG12 | 14:YF:197[E]:MET:HG2 | 1.81 | 0.62 |
| 14:YF:188[F]:VAL:HG12 | 14:YF:197[F]:MET:HG2 | 1.81 | 0.62 |
| 14:YF:262[A]:SER:O | 14:YF:289[A]:ARG:NH1 | 2.32 | 0.62 |
| 14:YF:60[A]:ILE:O | 14:YF:63[A]:LYS:N | 2.33 | 0.62 |
| 2:Z:121:LYS:HG2 | 2:Z:158:VAL:HG22 | 1.80 | 0.62 |
| 2:Z:398:SER:OG | 2:Z:399:ALA:N | 2.31 | 0.62 |
| 1:A:257:ILE:HG12 | 1:B:331:ILE:HD11 | 1.81 | 0.62 |
| 4:AA:111:ASN:ND2 | 4:AA:116:ILE:H | 1.98 | 0.62 |
| 5:AC:30:PHE:HE1 | 5:AE:30:PHE:HE1 | 1.48 | 0.62 |
| 5:AC:49:TRP:CZ3 | 5:AC:96:ARG:HD2 | 2.35 | 0.62 |
| 7:AJ:513:ARG:O | 7:BA:441:GLN:N | 2.23 | 0.62 |
| 7:BA:4:ASN:OD1 | 7:BA:15:TYR:OH | 2.17 | 0.62 |
| 7:AI:399:PHE:CD2 | 7:BA:514:PRO:HG2 | 2.35 | 0.62 |
| 2:BJ:326:VAL:HG21 | 2:BJ:413:TRP:HZ2 | 1.63 | 0.62 |
| 2:BJ:75:LEU:HA | 2:BJ:103:PHE:HA | 1.82 | 0.62 |
| 2:BJ:821:ILE:C | 2:BJ:824:GLN:HE22 | 2.01 | 0.62 |
| 2:BJ:925:LEU:HD12 | 2:BJ:993:LEU:HB3 | 1.80 | 0.62 |
| 2:C:628:HIS:O | 2:C:628:HIS:ND1 | 2.32 | 0.62 |
| 5:CF:184:THR:H | 5:CF:307:ASN:HD22 | 1.47 | 0.62 |
| 7:DB:194:ALA:HB2 | 7:DB:208:TYR:HB3 | 1.81 | 0.62 |
| 7:DD:162:PRO:HA | 7:DD:165:THR:HG22 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:399:PHE:CD2 | 7:DD:514:PRO:HG2 | 2.35 | 0.62 |
| 10:DH:222:ILE:HA | 10:DH:225:ILE:HG22 | 1.81 | 0.62 |
| 11:DI:43:TYR:HE2 | 11:DI:180:PHE:HB2 | 1.64 | 0.62 |
| 1:EB:87:SER:OG | 1:EB:230:ILE:O | 2.11 | 0.62 |
| 2:EC:75:LEU:HA | 2:EC:103:PHE:HA | 1.82 | 0.62 |
| 2:EC:993:LEU:HD12 | 2:EC:995:ASP:H | 1.63 | 0.62 |
| 5:EI:111:ALA:HB2 | 5:EI:117:ILE:HG23 | 1.80 | 0.62 |
| 5:EJ:194:LYS:HB2 | 5:EJ:243:GLN:HB2 | 1.82 | 0.62 |
| 5:FA:119:GLY:H | 5:FA:142:ARG:HH22 | 1.46 | 0.62 |
| 7:FE:193:LEU:HD13 | 7:FF:206:GLU:HG3 | 1.80 | 0.62 |
| 7:FF:81:LEU:O | 7:FF:85:LEU:N | 2.30 | 0.62 |
| 7:FG:66:VAL:HG21 | 7:FG:80:THR:HB | 1.82 | 0.62 |
| 1:GE:155:ARG:HA | 1:GE:161:TYR:HB3 | 1.81 | 0.62 |
| 1:GE:544:ASP:HB2 | 1:GE:576:ASP:HB2 | 1.80 | 0.62 |
| 3:GH:198:VAL:HG13 | 3:GH:202:ARG:HG3 | 1.81 | 0.62 |
| 4:H:111:ASN:ND2 | 4:H:116:ILE:H | 1.98 | 0.62 |
| 5:HB:206:PHE:HZ | 5:HB:221:GLU:HG2 | 1.63 | 0.62 |
| 6:HE:12:SER:HB3 | 6:HG:6:ASN:HB3 | 1.80 | 0.62 |
| 7:HH:140:GLY:HA2 | 7:HJ:129:PHE:CZ | 2.35 | 0.62 |
| 7:HH:310:ASN:OD1 | 7:HH:311:GLY:N | 2.32 | 0.62 |
| 7:HH:286:ASP:OD2 | 7:HJ:291:ARG:NH1 | 2.32 | 0.62 |
| 10:ID:222:ILE:HA | 10:ID:225:ILE:HG22 | 1.81 | 0.62 |
| 5:J:159:ILE:HG22 | 5:J:161:ASN:O | 1.99 | 0.62 |
| 6:L:13:ARG:HD2 | 6:N:10:VAL:HA | 1.81 | 0.62 |
| 7:Q:118:PRO:HA | 7:Q:121:PHE:HB3 | 1.82 | 0.62 |
| 10:U:132:SER:HA | 10:U:209:TRP:HE1 | 1.64 | 0.62 |
| 13:YA:61[D]:ILE:HA | 13:YB:76[D]:PRO:CA | 2.29 | 0.62 |
| 13:YB:50[D]:GLU:N | 13:YB:50[D]:GLU:OE2 | 2.33 | 0.62 |
| 14:YE:127[E]:ASP:OD1 | 14:YE:129[E]:GLY:N | 2.33 | 0.62 |
| 14:YE:17[D]:PHE:CE2 | 14:YE:28[D]:PHE:HB3 | 2.35 | 0.62 |
| 14:YE:66[F]:GLY:N | 14:YE:68[F]:GLU:OE2 | 2.32 | 0.62 |
| 14:YF:17[F]:PHE:CE2 | 14:YF:28[F]:PHE:HB3 | 2.35 | 0.62 |
| 14:YD:61[B]:HIS:CE1 | 14:YF:332[B]:GLN:HB3 | 2.34 | 0.62 |
| 14:YF:60[B]:ILE:O | 14:YF:63[B]:LYS:N | 2.32 | 0.62 |
| 14:YE:332[E]:GLN:HB3 | 14:YF:61[E]:HIS:CE1 | 2.34 | 0.62 |
| 14:YF:60[F]:ILE:O | 14:YF:63[F]:LYS:N | 2.33 | 0.62 |
| 2:Z:584:GLY:HA3 | 2:Z:597:TYR:OH | 1.98 | 0.62 |
| 2:Z:92:SER:OG | 2:Z:93:ASP:N | 2.32 | 0.62 |
| 1:A:358:GLN:HB2 | 1:A:379:LYS:HB3 | 1.80 | 0.62 |
| 1:A:539:ARG:HD3 | 1:A:580:LEU:HB3 | 1.80 | 0.62 |
| 6:AF:16:ASP:OD2 | 6:AF:45:LYS:NZ | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:386:THR:OG1 | 1:B:390:GLU:OE2 | 2.17 | 0.62 |
| 2:BJ:913:ILE:O | 2:BJ:914:ASN:ND2 | 2.33 | 0.62 |
| 2:C:312:THR:HG23 | 2:C:370:SER:HB3 | 1.81 | 0.62 |
| 3:CB:294:LYS:N | 3:CB:297:TYR:OH | 2.32 | 0.62 |
| 5:CF:196:ARG:NH2 | 5:CH:199:GLU:OE1 | 2.33 | 0.62 |
| 5:CF:409:SER:N | 5:CH:444:ASN:O | 2.32 | 0.62 |
| 5:CF:251:VAL:HG11 | 5:CH:254:TRP:CZ2 | 2.35 | 0.62 |
| 7:DB:134:SER:HB2 | 7:DD:143:LYS:HA | 1.82 | 0.62 |
| 7:DB:310:ASN:HA | 7:DC:316:THR:HB | 1.80 | 0.62 |
| 7:DD:66:VAL:HG21 | 7:DD:80:THR:HB | 1.82 | 0.62 |
| 12:BG:253:VAL:HG11 | 12:DJ:101:LEU:HD23 | 1.81 | 0.62 |
| 1:EA:90:VAL:O | 1:EA:94:GLN:N | 2.26 | 0.62 |
| 5:EI:304:ILE:HG23 | 5:EI:365:ILE:HD12 | 1.80 | 0.62 |
| 7:FE:418:ASP:OD1 | 7:FE:422:LYS:N | 2.30 | 0.62 |
| 7:FE:422:LYS:HB3 | 7:FF:504:ARG:HA | 1.82 | 0.62 |
| 7:FF:146:SER:HA | 7:FF:164:LYS:NZ | 2.14 | 0.62 |
| 8:FI:63:ASP:OD1 | 8:FI:64:ARG:N | 2.32 | 0.62 |
| 5:HC:153:LYS:HG2 | 5:HC:154:ILE:H | 1.64 | 0.62 |
| 5:HD:256:SER:O | 5:HD:258:TYR:N | 2.33 | 0.62 |
| 5:HD:328:LEU:HD12 | 5:HD:330:HIS:HD2 | 1.64 | 0.62 |
| 5:HB:356:TYR:HE1 | 6:HG:4:LEU:HD13 | 1.65 | 0.62 |
| 7:HJ:66:VAL:HG21 | 7:HJ:80:THR:HB | 1.82 | 0.62 |
| 10:ID:285:LEU:HA | 14:YD:215[F]:GLU:CG | 2.30 | 0.62 |
| 5:K:256:SER:O | 5:K:258:TYR:N | 2.33 | 0.62 |
| 7:P:212:PRO:HB2 | 7:Q:203:THR:HG22 | 1.81 | 0.62 |
| 7:Q:66:VAL:HG21 | 7:Q:80:THR:HB | 1.82 | 0.62 |
| 9:T:19:TRP:CE3 | 9:T:20:ASN:HB3 | 2.35 | 0.62 |
| 13:YA:61[A]:ILE:HA | 13:YB:76[A]:PRO:CA | 2.29 | 0.62 |
| 13:YB:50[B]:GLU:N | 13:YB:50[B]:GLU:OE2 | 2.33 | 0.62 |
| 13:YB:87[D]:LEU:HD21 | 13:YB:95[D]:ILE:HG23 | 1.80 | 0.62 |
| 14:YD:17[D]:PHE:CE2 | 14:YD:28[D]:PHE:HB3 | 2.35 | 0.62 |
| 14:YD:17[F]:PHE:CE2 | 14:YD:28[F]:PHE:HB3 | 2.35 | 0.62 |
| 14:YD:66[C]:GLY:N | 14:YD:68[C]:GLU:OE2 | 2.33 | 0.62 |
| 14:YE:60[A]:ILE:O | 14:YE:63[A]:LYS:N | 2.33 | 0.62 |
| 2:Z:957:PRO:O | 2:Z:958:MET:HG2 | 1.99 | 0.62 |
| 5:AD:221:GLU:OE2 | 5:AD:233:ARG:NH2 | 2.33 | 0.62 |
| 5:AD:31:ASP:O | 5:AD:35:TYR:N | 2.26 | 0.62 |
| 5:AD:198:ASN:HD22 | 5:AE:194:LYS:HD3 | 1.65 | 0.62 |
| 7:AJ:81:LEU:O | 7:AJ:85:LEU:N | 2.30 | 0.62 |
| 1:B:544:ASP:HB2 | 1:B:576:ASP:HB2 | 1.80 | 0.62 |
| 7:AJ:481:SER:OG | 7:BA:449:GLY:O | 2.18 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:211:VAL:N | 2:BJ:220:LYS:O | 2.27 | 0.62 |
| 2:C:75:LEU:HA | 2:C:103:PHE:HA | 1.82 | 0.62 |
| 2:C:872:SER:O | 2:C:873:SER:OG | 2.16 | 0.62 |
| 2:C:928:GLU:OE2 | 2:C:960:GLY:HA2 | 1.98 | 0.62 |
| 4:CC:103:LEU:O | 4:CE:69:LYS:NZ | 2.23 | 0.62 |
| 4:CD:42:PHE:O | 4:CD:62:HIS:ND1 | 2.27 | 0.62 |
| 5:CF:365:ILE:HB | 5:CF:366:PRO:CD | 2.29 | 0.62 |
| 5:CG:221:GLU:OE2 | 5:CG:233:ARG:NH2 | 2.33 | 0.62 |
| 3:D:292:ALA:HB1 | 3:D:297:TYR:CE2 | 2.35 | 0.62 |
| 6:DA:16:ASP:OD2 | 6:DA:45:LYS:NZ | 2.29 | 0.62 |
| 8:BB:14:ASP:HB2 | 8:DF:104:PRO:HD3 | 1.82 | 0.62 |
| 1:EA:506:LYS:O | 1:EA:509:SER:OG | 2.11 | 0.62 |
| 1:EA:96:ASN:HB3 | 1:EA:333:ARG:HB2 | 1.82 | 0.62 |
| 2:EC:180:ILE:HG13 | 2:EC:526:ILE:HD11 | 1.81 | 0.62 |
| 2:EC:326:VAL:HG21 | 2:EC:413:TRP:HZ2 | 1.64 | 0.62 |
| 2:EC:913:ILE:O | 2:EC:914:ASN:ND2 | 2.33 | 0.62 |
| 5:EI:472:TYR:HA | 5:EJ:416:ILE:HG23 | 1.82 | 0.62 |
| 5:FA:323:THR:HB | 5:FA:355:ASP:HB3 | 1.80 | 0.62 |
| 7:FG:4:ASN:OD1 | 7:FG:15:TYR:OH | 2.17 | 0.62 |
| 10:GA:222:ILE:HA | 10:GA:225:ILE:HG22 | 1.81 | 0.62 |
| 12:GC:253:VAL:HG11 | 12:IF:101:LEU:HD23 | 1.81 | 0.62 |
| 1:GE:495:PRO:O | 1:GE:498:GLY:N | 2.32 | 0.62 |
| 2:GF:110:PHE:HB2 | 2:GF:620:LYS:O | 2.00 | 0.62 |
| 2:GF:75:LEU:HA | 2:GF:103:PHE:HA | 1.82 | 0.62 |
| 4:GI:42:PHE:O | 4:GI:62:HIS:ND1 | 2.27 | 0.62 |
| 5:HB:62:ALA:HB1 | 5:HB:82:PRO:HG3 | 1.80 | 0.62 |
| 5:HC:103:ASN:OD1 | 5:HC:104:VAL:N | 2.33 | 0.62 |
| 5:HC:172:GLN:HG2 | 5:HC:173:GLY:H | 1.64 | 0.62 |
| 7:HJ:236:VAL:HG21 | 7:HJ:249:THR:HB | 1.81 | 0.62 |
| 7:O:229:LYS:HG3 | 7:O:243:VAL:HG12 | 1.81 | 0.62 |
| 7:O:310:ASN:OD1 | 7:O:311:GLY:N | 2.32 | 0.62 |
| 7:Q:236:VAL:HG21 | 7:Q:249:THR:HB | 1.81 | 0.62 |
| 8:R:43:ALA:O | 8:R:162:TRP:NE1 | 2.33 | 0.62 |
| 13:YB:313[A]:ASP:O | 13:YC:367[A]:PRO:HD3 | 2.00 | 0.62 |
| 13:YB:50[C]:GLU:N | 13:YB:50[C]:GLU:OE2 | 2.33 | 0.62 |
| 13:YB:58[F]:ILE:HG12 | 13:YB:97[F]:LEU:HD22 | 1.82 | 0.62 |
| 13:YB:418[A]:THR:HG21 | 13:YC:428[A]:GLY:HA3 | 1.80 | 0.62 |
| 13:YB:61[F]:ILE:HG12 | 13:YC:60[F]:PRO:HD2 | 1.81 | 0.62 |
| 14:YD:188[C]:VAL:HG12 | 14:YD:197[C]:MET:HG2 | 1.81 | 0.62 |
| 14:YD:17[B]:PHE:CE2 | 14:YD:28[B]:PHE:HB3 | 2.35 | 0.62 |
| 14:YD:332[D]:GLN:HB3 | 14:YE:61[D]:HIS:CE1 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:127[B]:ASP:OD1 | 14:YE:129[B]:GLY:N | 2.33 | 0.62 |
| 14:YE:60[E]:ILE:O | 14:YE:63[E]:LYS:N | 2.32 | 0.62 |
| 14:YF:127[A]:ASP:OD1 | 14:YF:129[A]:GLY:N | 2.33 | 0.62 |
| 14:YF:127[F]:ASP:OD1 | 14:YF:129[F]:GLY:N | 2.33 | 0.62 |
| 14:YF:60[C]:ILE:O | 14:YF:63[C]:LYS:N | 2.32 | 0.62 |
| 2:Z:415:ARG:HH12 | 2:Z:424:ARG:HH22 | 1.48 | 0.62 |
| 5:AC:184:THR:H | 5:AC:307:ASN:HD22 | 1.47 | 0.62 |
| 5:AD:63:GLU:HB2 | 5:AD:68:TYR:OH | 2.00 | 0.62 |
| 7:AJ:100:TYR:CE1 | 7:AJ:115:SER:HB2 | 2.34 | 0.62 |
| 7:AI:297:TYR:N | 7:BA:290:GLN:O | 2.26 | 0.62 |
| 1:BI:386:THR:OG1 | 1:BI:390:GLU:OE2 | 2.17 | 0.62 |
| 1:BH:341:THR:HG21 | 2:BJ:881:ARG:O | 1.99 | 0.62 |
| 2:C:110:PHE:HB2 | 2:C:620:LYS:O | 2.00 | 0.62 |
| 5:CG:212:PHE:CZ | 5:CG:230:ILE:HB | 2.35 | 0.62 |
| 5:CH:89:TYR:O | 5:CH:91:LYS:N | 2.33 | 0.62 |
| 7:DB:303:GLU:HA | 7:DC:309:ALA:HB3 | 1.80 | 0.62 |
| 7:DD:120:LYS:O | 7:DD:124:ALA:N | 2.32 | 0.62 |
| 7:DB:297:TYR:N | 7:DD:290:GLN:O | 2.25 | 0.62 |
| 1:EB:148:ARG:HH22 | 1:EB:196:GLN:HE22 | 1.46 | 0.62 |
| 1:EB:544:ASP:HB2 | 1:EB:576:ASP:HB2 | 1.80 | 0.62 |
| 5:FA:144:GLU:N | 5:FA:144:GLU:OE1 | 2.33 | 0.62 |
| 7:FE:229:LYS:HG3 | 7:FE:243:VAL:HG12 | 1.81 | 0.62 |
| 7:FE:310:ASN:OD1 | 7:FE:311:GLY:N | 2.32 | 0.62 |
| 7:FE:186:SER:O | 7:FG:192:GLN:NE2 | 2.33 | 0.62 |
| 8:DF:125:LYS:HG2 | 8:FI:79:HIS:HB2 | 1.82 | 0.62 |
| 9:FJ:19:TRP:CE3 | 9:FJ:20:ASN:HB3 | 2.35 | 0.62 |
| 1:GD:358:GLN:HB2 | 1:GD:379:LYS:HB3 | 1.80 | 0.62 |
| 3:GG:43:ARG:NH2 | 3:GG:47:TRP:HB3 | 2.15 | 0.62 |
| 5:HB:304:ILE:HG23 | 5:HB:365:ILE:HD12 | 1.80 | 0.62 |
| 5:HB:365:ILE:HB | 5:HB:366:PRO:CD | 2.29 | 0.62 |
| 7:HI:214:THR:HA | 7:HI:217:ASN:ND2 | 2.13 | 0.62 |
| 7:HH:186:SER:O | 7:HJ:192:GLN:NE2 | 2.33 | 0.62 |
| 7:HJ:476:ASP:OD1 | 7:HJ:479:ASN:ND2 | 2.30 | 0.62 |
| 11:IE:43:TYR:HE2 | 11:IE:180:PHE:HB2 | 1.64 | 0.62 |
| 5:J:221:GLU:OE2 | 5:J:233:ARG:NH2 | 2.33 | 0.62 |
| 5:J:212:PHE:CZ | 5:J:230:ILE:HB | 2.35 | 0.62 |
| 5:J:198:ASN:HD22 | 5:K:194:LYS:HD3 | 1.64 | 0.62 |
| 5:K:195:HIS:N | 5:K:197:GLY:O | 2.31 | 0.62 |
| 5:K:328:LEU:HD12 | 5:K:330:HIS:HD2 | 1.64 | 0.62 |
| 5:I:409:SER:N | 5:K:444:ASN:O | 2.32 | 0.62 |
| 7:O:230:LEU:HD23 | 7:O:246:THR:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:481:SER:OG | 7:Q:449:GLY:O | 2.18 | 0.62 |
| 13:YB:304[D]:TRP:O | 13:YB:308[D]:TYR:N | 2.32 | 0.62 |
| 13:YB:87[A]:LEU:HD21 | 13:YB:95[A]:ILE:HG23 | 1.80 | 0.62 |
| 13:YB:313[D]:ASP:O | 13:YC:367[D]:PRO:HD3 | 2.00 | 0.62 |
| 13:YC:572[C]:ILE:HD12 | 15:ZA:94[C]:VAL:HG22 | 1.81 | 0.62 |
| 13:YC:572[E]:ILE:HD12 | 15:ZA:94[E]:VAL:HG22 | 1.80 | 0.62 |
| 13:YA:47[C]:ILE:HG23 | 14:YD:123[C]:PRO:HG3 | 1.80 | 0.62 |
| 14:YD:127[D]:ASP:OD1 | 14:YD:129[D]:GLY:N | 2.33 | 0.62 |
| 14:YD:305[C]:ASP:OD1 | 14:YD:305[C]:ASP:N | 2.31 | 0.62 |
| 14:YD:66[B]:GLY:N | 14:YD:68[B]:GLU:OE2 | 2.33 | 0.62 |
| 14:YE:127[A]:ASP:OD1 | 14:YE:129[A]:GLY:N | 2.33 | 0.62 |
| 14:YE:127[C]:ASP:OD1 | 14:YE:129[C]:GLY:N | 2.33 | 0.62 |
| 14:YE:17[F]:PHE:CE2 | 14:YE:28[F]:PHE:HB3 | 2.35 | 0.62 |
| 14:YF:60[D]:ILE:O | 14:YF:63[D]:LYS:N | 2.32 | 0.62 |
| 14:YF:66[C]:GLY:N | 14:YF:68[C]:GLU:OE2 | 2.33 | 0.62 |
| 2:Z:458:ASP:HB3 | 2:Z:461:THR:OG1 | 1.99 | 0.62 |
| 5:AE:175:THR:O | 5:AE:232:LEU:N | 2.26 | 0.62 |
| 5:AE:89:TYR:O | 5:AE:91:LYS:N | 2.33 | 0.62 |
| 6:AF:13:ARG:HD2 | 6:AH:10:VAL:HA | 1.81 | 0.62 |
| 7:AI:310:ASN:HA | 7:AJ:316:THR:HB | 1.81 | 0.62 |
| 2:BJ:98:GLU:N | 2:BJ:98:GLU:OE1 | 2.30 | 0.62 |
| 2:C:87:GLN:HE21 | 3:D:158:GLY:HA2 | 1.65 | 0.62 |
| 5:CH:323:THR:HB | 5:CH:355:ASP:HB3 | 1.80 | 0.62 |
| 7:DB:230:LEU:HD23 | 7:DB:246:THR:HG22 | 1.81 | 0.62 |
| 7:DB:418:ASP:OD1 | 7:DB:422:LYS:N | 2.30 | 0.62 |
| 7:DC:163:LEU:HB3 | 7:DD:155:ASP:HA | 1.82 | 0.62 |
| 7:DD:365:GLY:HA3 | 7:DD:392:LEU:HD12 | 1.82 | 0.62 |
| 3:E:195:PRO:HD3 | 3:E:223:TRP:HD1 | 1.65 | 0.62 |
| 1:EB:495:PRO:O | 1:EB:498:GLY:N | 2.32 | 0.62 |
| 2:EC:121:LYS:HG2 | 2:EC:158:VAL:HG22 | 1.80 | 0.62 |
| 2:EC:415:ARG:HH12 | 2:EC:424:ARG:HH22 | 1.48 | 0.62 |
| 5:EJ:63:GLU:HB2 | 5:EJ:68:TYR:OH | 2.00 | 0.62 |
| 5:FA:214:SER:OG | 5:FA:222:LEU:O | 2.16 | 0.62 |
| 7:FF:263:VAL:O | 7:FG:255:SER:OG | 2.12 | 0.62 |
| 7:FF:36:ILE:HG21 | 7:FG:18:PHE:CZ | 2.34 | 0.62 |
| 7:FE:286:ASP:OD2 | 7:FG:291:ARG:NH1 | 2.33 | 0.62 |
| 8:DE:14:ASP:HB2 | 8:FI:104:PRO:HD3 | 1.82 | 0.62 |
| 1:GE:321:ASP:OD1 | 1:GE:322:ILE:N | 2.33 | 0.62 |
| 2:GF:913:ILE:O | 2:GF:914:ASN:ND2 | 2.33 | 0.62 |
| 4:GJ:111:ASN:ND2 | 4:GJ:116:ILE:H | 1.98 | 0.62 |
| 5:HD:214:SER:OG | 5:HD:222:LEU:O | 2.16 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:330:HIS:ND1 | 5:HD:355:ASP:HB2 | 2.14 | 0.62 |
| 7:HJ:120:LYS:O | 7:HJ:124:ALA:N | 2.32 | 0.62 |
| 11:IE:135:ASP:OD1 | 11:IE:136:LYS:N | 2.33 | 0.62 |
| 5:J:551:ILE:HD13 | 5:K:565:ILE:HD13 | 1.81 | 0.62 |
| 5:I:399:ILE:HG23 | 5:K:399:ILE:HD13 | 1.81 | 0.62 |
| 13:YA:58[F]:ILE:HG12 | 13:YA:97[F]:LEU:HD22 | 1.82 | 0.62 |
| 13:YB:193[A]:ASP:OD1 | 13:YB:197[A]:TYR:N | 2.32 | 0.62 |
| 13:YB:304[E]:TRP:O | 13:YB:308[E]:TYR:N | 2.33 | 0.62 |
| 13:YA:376[E]:PHE:CZ | 13:YB:447[E]:ASN:HB3 | 2.35 | 0.62 |
| 13:YB:442[D]:THR:HA | 13:YC:434[D]:THR:O | 1.99 | 0.62 |
| 13:YB:7[B]:ASN:ND2 | 13:YC:9[B]:ASN:HA | 2.14 | 0.62 |
| 14:YD:127[E]:ASP:OD1 | 14:YD:129[E]:GLY:N | 2.33 | 0.62 |
| 14:YD:245[B]:ARG:NE | 14:YD:246[B]:ASP:OD1 | 2.25 | 0.62 |
| 14:YD:60[A]:ILE:O | 14:YD:63[A]:LYS:N | 2.33 | 0.62 |
| 14:YD:60[B]:ILE:O | 14:YD:63[B]:LYS:N | 2.32 | 0.62 |
| 14:YD:66[F]:GLY:N | 14:YD:68[F]:GLU:OE2 | 2.32 | 0.62 |
| 14:YE:305[A]:ASP:OD1 | 14:YE:305[A]:ASP:N | 2.31 | 0.62 |
| 14:YE:66[A]:GLY:N | 14:YE:68[A]:GLU:OE2 | 2.33 | 0.62 |
| 2:Z:168:ILE:HG23 | 2:Z:169:GLY:N | 2.14 | 0.62 |
| 1:X:7:ASN:HD22 | 2:Z:634:PRO:HG2 | 1.64 | 0.62 |
| 1:A:21:PHE:CE2 | 1:A:75:VAL:HG11 | 2.35 | 0.61 |
| 5:AD:318:GLN:HE22 | 6:AF:8:ALA:N | 1.98 | 0.61 |
| 5:AC:472:TYR:HA | 5:AD:416:ILE:HG23 | 1.80 | 0.61 |
| 5:AE:313:PHE:HB3 | 5:AE:381:ILE:HG12 | 1.81 | 0.61 |
| 2:BJ:513:PHE:HB3 | 2:BJ:525:TRP:CZ3 | 2.33 | 0.61 |
| 1:BH:7:ASN:HD22 | 2:BJ:634:PRO:HG2 | 1.63 | 0.61 |
| 2:C:415:ARG:HH12 | 2:C:424:ARG:HH22 | 1.48 | 0.61 |
| 3:CB:226:GLU:N | 3:CB:226:GLU:OE1 | 2.31 | 0.61 |
| 5:CG:194:LYS:HB2 | 5:CG:243:GLN:HB2 | 1.82 | 0.61 |
| 5:CG:293:PHE:HD1 | 5:CG:298:LEU:HD11 | 1.65 | 0.61 |
| 5:CG:63:GLU:HB2 | 5:CG:68:TYR:OH | 2.00 | 0.61 |
| 5:CH:158:ASP:O | 5:CH:161:ASN:N | 2.31 | 0.61 |
| 9:DG:85:GLU:OE2 | 9:DG:87:ARG:NE | 2.29 | 0.61 |
| 1:EA:60:LEU:HD22 | 2:EC:671:TYR:CE1 | 2.35 | 0.61 |
| 5:EI:365:ILE:HB | 5:EI:366:PRO:CD | 2.29 | 0.61 |
| 5:EI:49:TRP:CZ3 | 5:EI:96:ARG:HD2 | 2.35 | 0.61 |
| 5:EJ:253:GLN:HE22 | 5:FA:249:ASP:HB3 | 1.65 | 0.61 |
| 5:EI:196:ARG:NH2 | 5:FA:199:GLU:OE1 | 2.33 | 0.61 |
| 5:FA:89:TYR:O | 5:FA:91:LYS:N | 2.33 | 0.61 |
| 10:GA:206:VAL:HG22 | 10:GA:347:THR:HG22 | 1.82 | 0.61 |
| 10:GA:132:SER:HA | 10:GA:209:TRP:HE1 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:DJ:253:VAL:HG11 | 12:GC:101:LEU:HD23 | 1.81 | 0.61 |
| 2:GF:312:THR:HG23 | 2:GF:370:SER:HB3 | 1.81 | 0.61 |
| 5:HD:144:GLU:OE1 | 5:HD:144:GLU:N | 2.33 | 0.61 |
| 7:HH:194:ALA:HB2 | 7:HH:208:TYR:HB3 | 1.81 | 0.61 |
| 8:IB:43:ALA:O | 8:IB:162:TRP:NE1 | 2.33 | 0.61 |
| 5:I:251:VAL:HG11 | 5:K:254:TRP:CZ2 | 2.34 | 0.61 |
| 8:R:63:ASP:OD1 | 8:R:64:ARG:N | 2.32 | 0.61 |
| 14:YD:66[A]:GLY:N | 14:YD:68[A]:GLU:OE2 | 2.33 | 0.61 |
| 14:YF:17[D]:PHE:CE2 | 14:YF:28[D]:PHE:HB3 | 2.35 | 0.61 |
| 5:AD:189:ASN:HD21 | 5:AE:150:GLN:NE2 | 1.98 | 0.61 |
| 5:AE:330:HIS:ND1 | 5:AE:355:ASP:HB2 | 2.14 | 0.61 |
| 7:AI:230:LEU:HD23 | 7:AI:246:THR:HG22 | 1.80 | 0.61 |
| 5:AE:196:ARG:NH1 | 7:AJ:5:THR:O | 2.33 | 0.61 |
| 7:BA:476:ASP:OD1 | 7:BA:479:ASN:ND2 | 2.30 | 0.61 |
| 2:C:360:ASN:C | 2:C:362:LYS:H | 2.02 | 0.61 |
| 2:C:913:ILE:O | 2:C:914:ASN:ND2 | 2.33 | 0.61 |
| 5:CF:49:TRP:CZ3 | 5:CF:96:ARG:HD2 | 2.35 | 0.61 |
| 5:CG:151:ILE:HD12 | 5:CG:152:ASP:H | 1.66 | 0.61 |
| 6:CI:12:SER:HB3 | 6:DA:6:ASN:HB3 | 1.82 | 0.61 |
| 6:AF:75:THR:HB | 7:DC:167:GLN:HE22 | 1.63 | 0.61 |
| 8:DF:43:ALA:O | 8:DF:162:TRP:NE1 | 2.33 | 0.61 |
| 11:DI:112:HIS:HB3 | 11:DI:150:LEU:HD13 | 1.81 | 0.61 |
| 11:DI:57:GLU:N | 11:DI:57:GLU:OE1 | 2.25 | 0.61 |
| 2:EC:87:GLN:HE21 | 3:ED:158:GLY:HA2 | 1.65 | 0.61 |
| 2:EC:940:GLY:O | 5:EI:21:LYS:NZ | 2.33 | 0.61 |
| 5:EJ:151:ILE:HD12 | 5:EJ:152:ASP:H | 1.66 | 0.61 |
| 7:FE:93:THR:HG22 | 7:FE:94:VAL:HG23 | 1.83 | 0.61 |
| 7:FG:236:VAL:HG21 | 7:FG:249:THR:HB | 1.81 | 0.61 |
| 11:GB:135:ASP:OD1 | 11:GB:136:LYS:N | 2.33 | 0.61 |
| 2:GF:872:SER:O | 2:GF:873:SER:OG | 2.16 | 0.61 |
| 4:HA:111:ASN:ND2 | 4:HA:116:ILE:H | 1.98 | 0.61 |
| 5:HC:221:GLU:OE2 | 5:HC:233:ARG:NH2 | 2.33 | 0.61 |
| 5:HC:63:GLU:HB2 | 5:HC:68:TYR:OH | 2.00 | 0.61 |
| 7:HI:481:SER:OG | 7:HJ:449:GLY:O | 2.18 | 0.61 |
| 5:I:397:ASP:O | 5:I:401:ASP:N | 2.19 | 0.61 |
| 5:I:472:TYR:HA | 5:J:416:ILE:HG23 | 1.81 | 0.61 |
| 5:I:459:ILE:HD11 | 5:K:463:ALA:HB2 | 1.82 | 0.61 |
| 7:P:146:SER:HA | 7:P:164:LYS:NZ | 2.14 | 0.61 |
| 7:Q:162:PRO:HA | 7:Q:165:THR:HG22 | 1.82 | 0.61 |
| 7:O:286:ASP:OD2 | 7:Q:291:ARG:NH1 | 2.33 | 0.61 |
| 1:X:21:PHE:CE2 | 1:X:75:VAL:HG11 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:193[B]:ASP:OD1 | 13:YB:197[B]:TYR:N | 2.33 | 0.61 |
| 13:YB:193[E]:ASP:OD1 | 13:YB:197[E]:TYR:N | 2.33 | 0.61 |
| 13:YB:304[B]:TRP:O | 13:YB:308[B]:TYR:N | 2.33 | 0.61 |
| 13:YA:376[D]:PHE:CZ | 13:YB:447[D]:ASN:HB3 | 2.35 | 0.61 |
| 13:YB:50[E]:GLU:OE2 | 13:YB:50[E]:GLU:N | 2.33 | 0.61 |
| 13:YB:66[F]:MET:SD | 13:YC:121[F]:TYR:HB3 | 2.41 | 0.61 |
| 13:YB:313[C]:ASP:O | 13:YC:367[C]:PRO:HD3 | 2.01 | 0.61 |
| 13:YC:50[B]:GLU:OE2 | 13:YC:50[B]:GLU:N | 2.33 | 0.61 |
| 13:YC:58[F]:ILE:HG12 | 13:YC:97[F]:LEU:HD22 | 1.82 | 0.61 |
| 13:YA:47[D]:ILE:HG23 | 14:YD:123[D]:PRO:HG3 | 1.81 | 0.61 |
| 14:YD:127[C]:ASP:OD1 | 14:YD:129[C]:GLY:N | 2.33 | 0.61 |
| 14:YD:188[A]:VAL:HG12 | 14:YD:197[A]:MET:HG2 | 1.81 | 0.61 |
| 14:YD:60[F]:ILE:O | 14:YD:63[F]:LYS:N | 2.33 | 0.61 |
| 14:YD:332[C]:GLN:HB3 | 14:YE:61[C]:HIS:CE1 | 2.34 | 0.61 |
| 14:YF:127[E]:ASP:OD1 | 14:YF:129[E]:GLY:N | 2.33 | 0.61 |
| 14:YF:312[D]:THR:OG1 | 14:YF:313[D]:ILE:N | 2.29 | 0.61 |
| 14:YF:66[B]:GLY:N | 14:YF:68[B]:GLU:OE2 | 2.33 | 0.61 |
| 14:YF:66[D]:GLY:N | 14:YF:68[D]:GLU:OE2 | 2.33 | 0.61 |
| 13:YC:572[F]:ILE:HD12 | 15:ZA:94[F]:VAL:HG22 | 1.82 | 0.61 |
| 5:AC:24:ILE:HG13 | 5:AE:7:ILE:HD11 | 1.82 | 0.61 |
| 6:AH:95:THR:N | 6:AH:174:TYR:O | 2.34 | 0.61 |
| 7:AI:286:ASP:OD2 | 7:BA:291:ARG:NH1 | 2.33 | 0.61 |
| 1:B:321:ASP:OD1 | 1:B:322:ILE:N | 2.33 | 0.61 |
| 8:BB:43:ALA:O | 8:BB:162:TRP:NE1 | 2.33 | 0.61 |
| 10:BE:132:SER:HA | 10:BE:209:TRP:HE1 | 1.64 | 0.61 |
| 2:BJ:415:ARG:HH12 | 2:BJ:424:ARG:HH22 | 1.48 | 0.61 |
| 2:BJ:703:TYR:O | 2:BJ:706:SER:N | 2.31 | 0.61 |
| 2:C:239:TYR:HB3 | 2:C:313:CYS:SG | 2.41 | 0.61 |
| 5:CF:234:GLN:NE2 | 7:DD:9:VAL:HG21 | 2.15 | 0.61 |
| 5:CF:356:TYR:HE1 | 6:DA:4:LEU:HD13 | 1.64 | 0.61 |
| 7:DB:229:LYS:HG3 | 7:DB:243:VAL:HG12 | 1.81 | 0.61 |
| 7:DB:473:LYS:HB3 | 7:DC:473:LYS:HD2 | 1.81 | 0.61 |
| 7:DB:192:GLN:NE2 | 7:DC:186:SER:O | 2.33 | 0.61 |
| 2:EC:110:PHE:HB2 | 2:EC:620:LYS:O | 2.00 | 0.61 |
| 3:EE:198:VAL:HG13 | 3:EE:202:ARG:HG3 | 1.81 | 0.61 |
| 4:EH:193:HIS:HB3 | 4:EH:196:GLU:HG3 | 1.83 | 0.61 |
| 5:EJ:172:GLN:HG2 | 5:EJ:173:GLY:H | 1.64 | 0.61 |
| 6:FC:16:ASP:OD2 | 6:FC:45:LYS:NZ | 2.29 | 0.61 |
| 5:EI:356:TYR:HE1 | 6:FD:4:LEU:HD13 | 1.65 | 0.61 |
| 7:FG:162:PRO:HA | 7:FG:165:THR:HG22 | 1.82 | 0.61 |
| 5:HB:49:TRP:CZ3 | 5:HB:96:ARG:HD2 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HF:95:THR:N | 6:HF:174:TYR:O | 2.34 | 0.61 |
| 7:HI:163:LEU:HB3 | 7:HJ:155:ASP:HA | 1.82 | 0.61 |
| 7:HI:193:LEU:HD21 | 7:HJ:207:GLY:HA2 | 1.81 | 0.61 |
| 7:HI:212:PRO:HB2 | 7:HJ:203:THR:HG22 | 1.81 | 0.61 |
| 7:HH:399:PHE:CD2 | 7:HJ:514:PRO:HG2 | 2.35 | 0.61 |
| 11:IE:57:GLU:OE1 | 11:IE:57:GLU:N | 2.25 | 0.61 |
| 5:J:212:PHE:HZ | 5:J:230:ILE:HB | 1.64 | 0.61 |
| 5:K:158:ASP:O | 5:K:161:ASN:N | 2.31 | 0.61 |
| 7:P:211:SER:H | 7:P:214:THR:HG1 | 1.47 | 0.61 |
| 7:Q:333:THR:OG1 | 7:Q:335:ASN:OD1 | 2.18 | 0.61 |
| 11:V:135:ASP:OD1 | 11:V:136:LYS:N | 2.33 | 0.61 |
| 13:YA:87[C]:LEU:HD21 | 13:YA:95[C]:ILE:HG23 | 1.80 | 0.61 |
| 13:YA:87[D]:LEU:HD21 | 13:YA:95[D]:ILE:HG23 | 1.80 | 0.61 |
| 13:YB:291[A]:LYS:HZ3 | 13:YC:362[A]:ASP:N | 1.98 | 0.61 |
| 13:YB:304[A]:TRP:O | 13:YB:308[A]:TYR:N | 2.32 | 0.61 |
| 13:YB:50[F]:GLU:OE2 | 13:YB:50[F]:GLU:N | 2.33 | 0.61 |
| 13:YC:65[E]:ALA:N | 13:YC:69[E]:ILE:O | 2.34 | 0.61 |
| 13:YB:61[C]:ILE:HD11 | 13:YC:72[C]:SER:O | 1.99 | 0.61 |
| 14:YD:118[C]:LEU:HD23 | 14:YD:139[C]:ILE:HD13 | 1.82 | 0.61 |
| 14:YD:312[B]:THR:OG1 | 14:YD:313[B]:ILE:N | 2.29 | 0.61 |
| 14:YE:66[C]:GLY:N | 14:YE:68[C]:GLU:OE2 | 2.33 | 0.61 |
| 14:YE:66[D]:GLY:N | 14:YE:68[D]:GLU:OE2 | 2.33 | 0.61 |
| 4:AB:111:ASN:ND2 | 4:AB:116:ILE:H | 1.98 | 0.61 |
| 5:AE:186:TYR:OH | 5:AE:190:ASN:O | 2.12 | 0.61 |
| 5:AE:256:SER:O | 5:AE:258:TYR:N | 2.33 | 0.61 |
| 7:AI:229:LYS:HG3 | 7:AI:243:VAL:HG12 | 1.81 | 0.61 |
| 7:AJ:263:VAL:O | 7:BA:255:SER:OG | 2.15 | 0.61 |
| 1:B:448:TYR:HA | 1:B:452:VAL:HG12 | 1.83 | 0.61 |
| 11:BF:135:ASP:CG | 11:BF:136:LYS:H | 2.02 | 0.61 |
| 2:BJ:514:PHE:HB3 | 2:BJ:523:ARG:HB3 | 1.82 | 0.61 |
| 2:BJ:59:LEU:HD13 | 2:BJ:67:PHE:CE2 | 2.36 | 0.61 |
| 2:C:211:VAL:N | 2:C:220:LYS:O | 2.27 | 0.61 |
| 2:C:292:GLU:N | 2:C:292:GLU:OE1 | 2.34 | 0.61 |
| 5:CF:206:PHE:CZ | 5:CF:221:GLU:HG2 | 2.35 | 0.61 |
| 5:CG:260:ARG:O | 5:CG:261:ARG:NH1 | 2.33 | 0.61 |
| 5:CH:144:GLU:N | 5:CH:144:GLU:OE1 | 2.33 | 0.61 |
| 7:DC:193:LEU:HD21 | 7:DD:207:GLY:HA2 | 1.81 | 0.61 |
| 9:DG:19:TRP:CE3 | 9:DG:20:ASN:HB3 | 2.35 | 0.61 |
| 10:DH:206:VAL:HG22 | 10:DH:347:THR:HG22 | 1.82 | 0.61 |
| 3:E:219:ASP:OD1 | 3:E:221:THR:N | 2.32 | 0.61 |
| 2:EC:628:HIS:O | 2:EC:628:HIS:ND1 | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:184:THR:H | 5:EI:307:ASN:HD22 | 1.47 | 0.61 |
| 4:F:43:GLY:O | 4:F:68:GLN:NE2 | 2.32 | 0.61 |
| 5:EI:43:PRO:HG3 | 5:FA:33:LEU:HA | 1.83 | 0.61 |
| 7:FE:447:HIS:HD2 | 7:FF:447:HIS:CD2 | 2.17 | 0.61 |
| 7:FE:512:THR:HA | 7:FF:442:MET:HA | 1.82 | 0.61 |
| 7:FF:163:LEU:HB3 | 7:FG:155:ASP:HA | 1.83 | 0.61 |
| 12:GC:216:PHE:HE1 | 12:GC:218:MET:HE3 | 1.64 | 0.61 |
| 1:GD:21:PHE:CE2 | 1:GD:75:VAL:HG11 | 2.35 | 0.61 |
| 5:HB:206:PHE:CZ | 5:HB:221:GLU:HG2 | 2.35 | 0.61 |
| 5:HC:317:LEU:HD13 | 5:HD:312:ARG:HH22 | 1.65 | 0.61 |
| 5:HD:119:GLY:H | 5:HD:142:ARG:HH22 | 1.46 | 0.61 |
| 5:HC:147:LYS:HB2 | 5:HD:153:LYS:HB2 | 1.82 | 0.61 |
| 7:P:167:GLN:HE22 | 6:HE:75:THR:HB | 1.65 | 0.61 |
| 7:HH:309:ALA:HB3 | 7:HJ:303:GLU:HA | 1.83 | 0.61 |
| 7:HH:326:ILE:HG23 | 7:HJ:323:GLY:HA2 | 1.82 | 0.61 |
| 12:IF:161:SER:HA | 12:IF:240:ASP:HA | 1.83 | 0.61 |
| 5:J:260:ARG:O | 5:J:261:ARG:NH1 | 2.33 | 0.61 |
| 5:K:144:GLU:OE1 | 5:K:144:GLU:N | 2.33 | 0.61 |
| 5:J:189:ASN:HD21 | 5:K:150:GLN:NE2 | 1.98 | 0.61 |
| 6:L:93:THR:HG22 | 6:L:94:VAL:HG23 | 3.79 | 0.61 |
| 7:O:326:ILE:HG23 | 7:Q:323:GLY:HA2 | 1.81 | 0.61 |
| 7:Q:365:GLY:HA3 | 7:Q:392:LEU:HD12 | 1.83 | 0.61 |
| 1:X:229:THR:OG1 | 1:X:231:ASP:OD1 | 2.18 | 0.61 |
| 13:YA:72[A]:SER:O | 13:YC:61[A]:ILE:HD11 | 2.00 | 0.61 |
| 13:YA:57[C]:VAL:CG1 | 13:YA:76[C]:PRO:HD3 | 2.31 | 0.61 |
| 13:YB:563[D]:GLY:N | 13:YC:555[D]:ALA:O | 2.30 | 0.61 |
| 13:YB:66[D]:MET:SD | 13:YC:121[D]:TYR:HB3 | 2.41 | 0.61 |
| 13:YC:193[C]:ASP:OD1 | 13:YC:197[C]:TYR:N | 2.31 | 0.61 |
| 13:YC:572[D]:ILE:HD12 | 15:ZA:94[D]:VAL:HG22 | 1.81 | 0.61 |
| 14:YD:188[B]:VAL:HG12 | 14:YD:197[B]:MET:HG2 | 1.81 | 0.61 |
| 14:YE:188[E]:VAL:HG12 | 14:YE:197[E]:MET:HG2 | 1.81 | 0.61 |
| 14:YE:245[F]:ARG:NE | 14:YE:246[F]:ASP:OD1 | 2.26 | 0.61 |
| 14:YE:294[E]:GLU:O | 14:YE:297[E]:ARG:N | 2.34 | 0.61 |
| 14:YE:360[C]:ASN:HD22 | 14:YE:360[C]:ASN:N | 1.97 | 0.61 |
| 14:YF:305[E]:ASP:OD1 | 14:YF:305[E]:ASP:N | 2.32 | 0.61 |
| 2:Z:110:PHE:HB2 | 2:Z:620:LYS:O | 2.00 | 0.61 |
| 2:Z:364:VAL:HG11 | 2:Z:390:PRO:HB3 | 1.82 | 0.61 |
| 4:AA:193:HIS:HB3 | 4:AA:196:GLU:HG3 | 1.82 | 0.61 |
| 4:AA:53:GLY:HA2 | 4:AA:59:GLN:H | 1.66 | 0.61 |
| 5:AC:206:PHE:CZ | 5:AC:221:GLU:HG2 | 2.35 | 0.61 |
| 1:BH:41:ASN:OD1 | 1:BH:42:GLU:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:321:ASP:OD1 | 1:BI:322:ILE:N | 2.33 | 0.61 |
| 2:BJ:159:ASP:HB3 | 2:BJ:162:SER:H | 1.65 | 0.61 |
| 2:BJ:364:VAL:HG11 | 2:BJ:390:PRO:HB3 | 1.82 | 0.61 |
| 2:BJ:376:PHE:HZ | 2:BJ:441:VAL:HG11 | 1.65 | 0.61 |
| 2:BJ:143:MET:HG2 | 2:BJ:544:VAL:HG13 | 1.82 | 0.61 |
| 2:C:950:GLU:N | 2:C:950:GLU:OE1 | 2.24 | 0.61 |
| 3:CA:292:ALA:HB1 | 3:CA:297:TYR:CE2 | 2.35 | 0.61 |
| 4:CE:111:ASN:ND2 | 4:CE:116:ILE:H | 1.98 | 0.61 |
| 4:CC:7:LYS:HB2 | 4:CE:39:TYR:CD1 | 2.36 | 0.61 |
| 5:CF:407:TYR:OH | 5:CH:403:THR:HA | 2.00 | 0.61 |
| 5:CG:103:ASN:N | 5:CG:127:ASN:O | 2.31 | 0.61 |
| 5:CH:290:SER:CB | 5:CH:371:PHE:H | 2.14 | 0.61 |
| 5:CH:330:HIS:ND1 | 5:CH:355:ASP:HB2 | 2.14 | 0.61 |
| 6:CI:95:THR:N | 6:CI:174:TYR:O | 2.34 | 0.61 |
| 6:DA:95:THR:N | 6:DA:174:TYR:O | 2.34 | 0.61 |
| 7:DC:146:SER:HA | 7:DC:164:LYS:NZ | 2.14 | 0.61 |
| 2:EC:292:GLU:OE1 | 2:EC:292:GLU:N | 2.34 | 0.61 |
| 2:EC:59:LEU:HD13 | 2:EC:67:PHE:CE2 | 2.36 | 0.61 |
| 3:ED:43:ARG:NH2 | 3:ED:47:TRP:HB3 | 2.15 | 0.61 |
| 3:EE:226:GLU:OE1 | 3:EE:226:GLU:N | 2.31 | 0.61 |
| 2:BJ:529:SER:H | 3:EE:233:GLN:HE22 | 1.46 | 0.61 |
| 3:EE:294:LYS:N | 3:EE:297:TYR:OH | 2.32 | 0.61 |
| 4:EF:53:GLY:HA2 | 4:EF:59:GLN:H | 1.66 | 0.61 |
| 4:EG:53:GLY:HA2 | 4:EG:59:GLN:H | 1.66 | 0.61 |
| 5:EI:72:THR:OG1 | 5:EI:101:THR:O | 2.19 | 0.61 |
| 5:EI:89:TYR:O | 5:EI:91:LYS:N | 2.34 | 0.61 |
| 5:EJ:95:ALA:HB3 | 5:EJ:133:LEU:HB2 | 1.82 | 0.61 |
| 5:EJ:371:PHE:CZ | 5:EJ:373:SER:HB3 | 2.34 | 0.61 |
| 4:F:7:LYS:HB2 | 4:H:39:TYR:CD1 | 2.35 | 0.61 |
| 5:FA:256:SER:O | 5:FA:258:TYR:N | 2.33 | 0.61 |
| 1:GD:229:THR:OG1 | 1:GD:231:ASP:OD1 | 2.19 | 0.61 |
| 2:GF:150:SER:OG | 2:GF:151:PHE:N | 2.33 | 0.61 |
| 2:GF:628:HIS:O | 2:GF:628:HIS:ND1 | 2.32 | 0.61 |
| 3:GG:43:ARG:HH22 | 3:GG:47:TRP:HB3 | 1.66 | 0.61 |
| 5:I:95:ALA:HB3 | 5:I:133:LEU:HB2 | 1.83 | 0.61 |
| 5:I:365:ILE:HB | 5:I:366:PRO:CD | 2.29 | 0.61 |
| 5:J:31:ASP:O | 5:J:35:TYR:N | 2.26 | 0.61 |
| 5:J:60:LEU:HG | 5:J:79:ILE:HG22 | 1.82 | 0.61 |
| 5:I:407:TYR:OH | 5:K:403:THR:HA | 2.01 | 0.61 |
| 1:X:539:ARG:HD3 | 1:X:580:LEU:HB3 | 1.80 | 0.61 |
| 13:YC:437[F]:ASN:HB3 | 13:YC:439[F]:TYR:HE1 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:118[D]:LEU:HD23 | 14:YD:139[D]:ILE:HD13 | 1.83 | 0.61 |
| 14:YD:360[E]:ASN:HD22 | 14:YD:360[E]:ASN:N | 1.98 | 0.61 |
| 14:YE:118[B]:LEU:HD23 | 14:YE:139[B]:ILE:HD13 | 1.83 | 0.61 |
| 14:YE:188[F]:VAL:HG12 | 14:YE:197[F]:MET:HG2 | 1.81 | 0.61 |
| 14:YF:188[D]:VAL:HG12 | 14:YF:197[D]:MET:HG2 | 1.81 | 0.61 |
| 14:YF:66[E]:GLY:N | 14:YF:68[E]:GLU:OE2 | 2.33 | 0.61 |
| 2:Z:768:TYR:OH | 2:Z:814:HIS:O | 2.17 | 0.61 |
| 2:Z:913:ILE:O | 2:Z:914:ASN:ND2 | 2.33 | 0.61 |
| 5:AC:196:ARG:NH2 | 5:AE:199:GLU:OE1 | 2.34 | 0.61 |
| 5:AC:89:TYR:O | 5:AC:91:LYS:N | 2.34 | 0.61 |
| 5:AD:194:LYS:HB2 | 5:AD:243:GLN:HB2 | 1.82 | 0.61 |
| 5:AD:293:PHE:HD1 | 5:AD:298:LEU:HD11 | 1.66 | 0.61 |
| 7:AI:140:GLY:HA2 | 7:BA:129:PHE:CZ | 2.35 | 0.61 |
| 1:B:238:PHE:CE1 | 1:B:262:PRO:HD2 | 2.36 | 0.61 |
| 7:BA:27:PRO:HA | 7:BA:29:ILE:HD11 | 1.82 | 0.61 |
| 7:AI:326:ILE:HG23 | 7:BA:323:GLY:HA2 | 1.82 | 0.61 |
| 1:BH:21:PHE:CE2 | 1:BH:75:VAL:HG11 | 2.35 | 0.61 |
| 2:BJ:292:GLU:N | 2:BJ:292:GLU:OE1 | 2.34 | 0.61 |
| 5:CF:95:ALA:HB3 | 5:CF:133:LEU:HB2 | 1.83 | 0.61 |
| 5:CF:484:GLY:N | 5:CG:489:GLY:O | 2.28 | 0.61 |
| 5:CG:600:ARG:NE | 5:CG:602:ALA:O | 2.32 | 0.61 |
| 5:CH:174:GLN:HE21 | 5:CH:177:PHE:HE1 | 1.49 | 0.61 |
| 7:DC:71:ASN:O | 7:DC:73:THR:HG22 | 2.01 | 0.61 |
| 3:ED:228:ASN:OD1 | 3:ED:229:LEU:N | 2.34 | 0.61 |
| 5:EJ:221:GLU:OE2 | 5:EJ:233:ARG:NH2 | 2.33 | 0.61 |
| 5:EJ:293:PHE:HD1 | 5:EJ:298:LEU:HD11 | 1.65 | 0.61 |
| 4:F:106:CYS:SG | 4:F:149:ARG:NH2 | 2.67 | 0.61 |
| 4:F:53:GLY:HA2 | 4:F:59:GLN:H | 1.66 | 0.61 |
| 7:FG:27:PRO:HA | 7:FG:29:ILE:HD11 | 1.81 | 0.61 |
| 8:FH:43:ALA:O | 8:FH:162:TRP:NE1 | 2.33 | 0.61 |
| 12:DJ:211:HIS:CE1 | 12:GC:167:GLU:HA | 2.35 | 0.61 |
| 5:HB:95:ALA:HB3 | 5:HB:133:LEU:HB2 | 1.83 | 0.61 |
| 5:HC:194:LYS:HB2 | 5:HC:243:GLN:HB2 | 1.82 | 0.61 |
| 7:HH:93:THR:HG22 | 7:HH:94:VAL:HG23 | 1.83 | 0.61 |
| 5:I:36:GLU:HA | 5:I:50:LYS:HZ1 | 1.65 | 0.61 |
| 5:I:49:TRP:CZ3 | 5:I:96:ARG:HD2 | 2.35 | 0.61 |
| 10:ID:132:SER:HA | 10:ID:209:TRP:HE1 | 1.65 | 0.61 |
| 5:J:293:PHE:HD1 | 5:J:298:LEU:HD11 | 1.66 | 0.61 |
| 7:Q:120:LYS:O | 7:Q:124:ALA:N | 2.32 | 0.61 |
| 7:P:36:ILE:HG21 | 7:Q:18:PHE:CZ | 2.35 | 0.61 |
| 10:U:42:ARG:HG3 | 10:U:58:TYR:HB3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:238:PHE:CE1 | 1:Y:262:PRO:HD2 | 2.36 | 0.61 |
| 1:Y:448:TYR:HA | 1:Y:452:VAL:HG12 | 1.83 | 0.61 |
| 13:YA:376[F]:PHE:CZ | 13:YB:447[F]:ASN:HB3 | 2.35 | 0.61 |
| 13:YA:567[D]:ILE:O | 13:YC:575[D]:GLY:N | 2.34 | 0.61 |
| 13:YB:66[C]:MET:SD | 13:YC:121[C]:TYR:HB3 | 2.40 | 0.61 |
| 13:YC:57[A]:VAL:HB | 13:YC:76[A]:PRO:HB3 | 1.83 | 0.61 |
| 14:YD:294[D]:GLU:O | 14:YD:297[D]:ARG:N | 2.34 | 0.61 |
| 14:YD:294[E]:GLU:O | 14:YD:297[E]:ARG:N | 2.34 | 0.61 |
| 14:YE:118[A]:LEU:HD23 | 14:YE:139[A]:ILE:HD13 | 1.83 | 0.61 |
| 14:YE:60[F]:ILE:O | 14:YE:63[F]:LYS:N | 2.33 | 0.61 |
| 14:YD:332[B]:GLN:HB3 | 14:YE:61[B]:HIS:CE1 | 2.35 | 0.61 |
| 14:YF:188[C]:VAL:HG12 | 14:YF:197[C]:MET:HG2 | 1.81 | 0.61 |
| 14:YF:294[C]:GLU:O | 14:YF:297[C]:ARG:N | 2.34 | 0.61 |
| 14:YF:184[C]:LYS:HE3 | 14:YF:367[C]:ILE:HG21 | 1.83 | 0.61 |
| 14:YF:66[A]:GLY:N | 14:YF:68[A]:GLU:OE2 | 2.33 | 0.61 |
| 2:Z:145:ALA:HB2 | 2:Z:542:THR:HB | 1.83 | 0.61 |
| 1:A:242:GLU:O | 1:A:256:TYR:OH | 2.16 | 0.61 |
| 1:A:96:ASN:HB3 | 1:A:333:ARG:HB2 | 1.82 | 0.61 |
| 7:AI:184:THR:OG1 | 7:AI:187:ASP:N | 2.34 | 0.61 |
| 1:B:352:ARG:HG3 | 1:B:395:TYR:CZ | 2.36 | 0.61 |
| 1:B:495:PRO:O | 1:B:498:GLY:N | 2.32 | 0.61 |
| 5:AD:196:ARG:HE | 7:BA:5:THR:HG23 | 1.65 | 0.61 |
| 8:BC:125:LYS:HG2 | 8:DF:79:HIS:HB2 | 1.82 | 0.61 |
| 2:BJ:110:PHE:HB2 | 2:BJ:620:LYS:O | 2.00 | 0.61 |
| 2:BJ:398:SER:OG | 2:BJ:399:ALA:N | 2.31 | 0.61 |
| 2:BJ:423:GLU:OE1 | 2:BJ:423:GLU:N | 2.30 | 0.61 |
| 4:CD:193:HIS:HB3 | 4:CD:196:GLU:HG3 | 1.83 | 0.61 |
| 5:CF:30:PHE:HE1 | 5:CH:30:PHE:HE1 | 1.49 | 0.61 |
| 7:DD:118:PRO:HA | 7:DD:121:PHE:HB3 | 1.82 | 0.61 |
| 1:EA:227:ARG:HD3 | 1:EA:237:TYR:CE2 | 2.36 | 0.61 |
| 1:EB:238:PHE:CE1 | 1:EB:262:PRO:HD2 | 2.36 | 0.61 |
| 1:EB:321:ASP:OD1 | 1:EB:322:ILE:N | 2.33 | 0.61 |
| 3:ED:253:LEU:HD12 | 3:ED:326:GLU:HB2 | 1.83 | 0.61 |
| 4:EG:193:HIS:HB3 | 4:EG:196:GLU:HG3 | 1.83 | 0.61 |
| 4:EF:7:LYS:NZ | 4:EH:36:ASN:OD1 | 2.25 | 0.61 |
| 5:EJ:103:ASN:OD1 | 5:EJ:104:VAL:N | 2.33 | 0.61 |
| 5:EJ:260:ARG:O | 5:EJ:261:ARG:NH1 | 2.33 | 0.61 |
| 6:FB:73:ASN:HA | 6:FD:70:ILE:HG12 | 1.82 | 0.61 |
| 7:FE:134:SER:HB2 | 7:FG:143:LYS:HA | 1.82 | 0.61 |
| 7:FG:333:THR:OG1 | 7:FG:335:ASN:OD1 | 2.18 | 0.61 |
| 1:GD:41:ASN:OD1 | 1:GD:42:GLU:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:703:TYR:O | 2:GF:706:SER:N | 2.31 | 0.61 |
| 3:GG:253:LEU:HD12 | 3:GG:326:GLU:HB2 | 1.83 | 0.61 |
| 3:GH:46:PRO:HA | 3:GH:270:ARG:HH21 | 1.65 | 0.61 |
| 4:HA:193:HIS:HB3 | 4:HA:196:GLU:HG3 | 1.83 | 0.61 |
| 5:HB:72:THR:OG1 | 5:HB:101:THR:O | 2.19 | 0.61 |
| 5:HC:159:ILE:HG22 | 5:HC:161:ASN:O | 1.99 | 0.61 |
| 5:CH:362:GLU:OE2 | 7:HH:473:LYS:HE2 | 2.00 | 0.61 |
| 7:HJ:162:PRO:HA | 7:HJ:165:THR:HG22 | 1.82 | 0.61 |
| 5:HB:234:GLN:NE2 | 7:HJ:9:VAL:HG21 | 2.15 | 0.61 |
| 10:ID:42:ARG:HG3 | 10:ID:58:TYR:HB3 | 1.83 | 0.61 |
| 5:K:174:GLN:HE21 | 5:K:177:PHE:HE1 | 1.49 | 0.61 |
| 13:YA:438[F]:LEU:HD22 | 13:YC:442[F]:THR:HG21 | 1.83 | 0.61 |
| 13:YB:563[E]:GLY:N | 13:YC:555[E]:ALA:O | 2.30 | 0.61 |
| 13:YB:57[C]:VAL:CG1 | 13:YB:76[C]:PRO:HD3 | 2.30 | 0.61 |
| 13:YB:65[E]:ALA:N | 13:YB:69[E]:ILE:O | 2.34 | 0.61 |
| 13:YB:291[E]:LYS:HZ3 | 13:YC:362[E]:ASP:N | 1.98 | 0.61 |
| 14:YE:66[E]:GLY:N | 14:YE:68[E]:GLU:OE2 | 2.33 | 0.61 |
| 14:YE:70[F]:ILE:O | 14:YE:88[F]:TYR:N | 2.34 | 0.61 |
| 14:YF:245[D]:ARG:NE | 14:YF:246[D]:ASP:OD1 | 2.25 | 0.61 |
| 2:Z:159:ASP:HB3 | 2:Z:162:SER:H | 1.65 | 0.61 |
| 2:Z:514:PHE:HB3 | 2:Z:523:ARG:HB3 | 1.82 | 0.61 |
| 1:A:227:ARG:HD3 | 1:A:237:TYR:CE2 | 2.36 | 0.61 |
| 5:AD:103:ASN:OD1 | 5:AD:104:VAL:N | 2.33 | 0.61 |
| 7:AI:309:ALA:HB3 | 7:BA:303:GLU:HA | 1.83 | 0.61 |
| 7:BA:236:VAL:HG21 | 7:BA:249:THR:HB | 1.81 | 0.61 |
| 2:BJ:752:TYR:OH | 2:BJ:878:ASP:OD2 | 2.11 | 0.61 |
| 3:CA:228:ASN:OD1 | 3:CA:229:LEU:N | 2.34 | 0.61 |
| 5:CF:89:TYR:O | 5:CF:91:LYS:N | 2.34 | 0.61 |
| 5:CH:119:GLY:H | 5:CH:142:ARG:HH22 | 1.46 | 0.61 |
| 5:CH:313:PHE:HB3 | 5:CH:381:ILE:HG12 | 1.81 | 0.61 |
| 3:D:43:ARG:NH2 | 3:D:47:TRP:HB3 | 2.15 | 0.61 |
| 7:DB:93:THR:HG22 | 7:DB:94:VAL:HG23 | 1.83 | 0.61 |
| 6:AF:218:THR:HB | 7:DC:205:ARG:HH12 | 1.65 | 0.61 |
| 11:DI:131:TYR:O | 11:DI:148:GLY:N | 2.25 | 0.61 |
| 11:DI:135:ASP:OD1 | 11:DI:136:LYS:N | 2.33 | 0.61 |
| 12:DJ:161:SER:HA | 12:DJ:240:ASP:HA | 1.83 | 0.61 |
| 3:E:226:GLU:OE1 | 3:E:226:GLU:N | 2.31 | 0.61 |
| 1:EB:455:PHE:CD1 | 1:EB:639:LEU:HD12 | 2.35 | 0.61 |
| 4:EF:111:ASN:ND2 | 4:EF:116:ILE:H | 1.98 | 0.61 |
| 5:EI:34:TYR:O | 5:EI:38:GLY:N | 2.26 | 0.61 |
| 5:FA:419:ASP:OD1 | 5:FA:420:VAL:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FB:95:THR:N | 6:FB:174:TYR:O | 2.34 | 0.61 |
| 7:FF:422:LYS:NZ | 7:FG:498:SER:O | 2.33 | 0.61 |
| 8:FH:162:TRP:O | 8:IA:95:GLN:NE2 | 2.33 | 0.61 |
| 8:FI:43:ALA:O | 8:FI:162:TRP:NE1 | 2.33 | 0.61 |
| 4:G:42:PHE:O | 4:G:62:HIS:ND1 | 2.27 | 0.61 |
| 2:GF:981:GLN:HG2 | 2:GF:982:LEU:N | 2.16 | 0.61 |
| 4:HA:53:GLY:HA2 | 4:HA:59:GLN:H | 1.66 | 0.61 |
| 5:HB:323:THR:HG23 | 5:HB:359:GLU:HB2 | 1.83 | 0.61 |
| 5:HC:316:ILE:HG23 | 5:HD:315:GLY:HA3 | 1.82 | 0.61 |
| 7:HJ:333:THR:OG1 | 7:HJ:335:ASN:OD1 | 2.18 | 0.61 |
| 5:I:206:PHE:CZ | 5:I:221:GLU:HG2 | 2.35 | 0.61 |
| 5:J:95:ALA:HB3 | 5:J:133:LEU:HB2 | 1.82 | 0.61 |
| 5:J:146:VAL:HB | 5:K:153:LYS:HA | 1.83 | 0.61 |
| 5:K:214:SER:OG | 5:K:222:LEU:O | 2.16 | 0.61 |
| 5:K:89:TYR:O | 5:K:91:LYS:N | 2.33 | 0.61 |
| 7:O:93:THR:HG22 | 7:O:94:VAL:HG23 | 1.83 | 0.61 |
| 7:P:167:GLN:NE2 | 6:HE:77:VAL:HG23 | 2.16 | 0.61 |
| 7:Q:27:PRO:HA | 7:Q:29:ILE:HD11 | 1.81 | 0.61 |
| 13:YA:376[B]:PHE:CZ | 13:YB:447[B]:ASN:HB3 | 2.35 | 0.61 |
| 13:YA:567[C]:ILE:O | 13:YC:575[C]:GLY:N | 2.34 | 0.61 |
| 13:YB:313[F]:ASP:O | 13:YC:367[F]:PRO:HD3 | 2.00 | 0.61 |
| 13:YB:57[A]:VAL:HB | 13:YB:76[A]:PRO:HB3 | 1.83 | 0.61 |
| 14:YD:184[A]:LYS:HE3 | 14:YD:367[A]:ILE:HG21 | 1.83 | 0.61 |
| 14:YE:294[C]:GLU:O | 14:YE:297[C]:ARG:N | 2.34 | 0.61 |
| 14:YE:184[C]:LYS:HE3 | 14:YE:367[C]:ILE:HG21 | 1.83 | 0.61 |
| 14:YF:125[B]:PHE:CE2 | 14:YF:134[B]:GLU:HG3 | 2.30 | 0.61 |
| 2:Z:292:GLU:OE1 | 2:Z:292:GLU:N | 2.34 | 0.61 |
| 1:A:126:PRO:HD2 | 1:A:292:LEU:HD21 | 1.82 | 0.61 |
| 5:AC:290:SER:CB | 5:AC:370:HIS:HA | 2.31 | 0.61 |
| 5:AD:213:GLY:HA2 | 5:AD:221:GLU:HB2 | 1.83 | 0.61 |
| 5:AE:174:GLN:HE21 | 5:AE:177:PHE:HE1 | 1.49 | 0.61 |
| 5:AD:551:ILE:HD13 | 5:AE:565:ILE:HD13 | 1.81 | 0.61 |
| 7:AJ:453:GLU:OE2 | 7:AJ:471:THR:N | 2.31 | 0.61 |
| 7:AI:160:MET:SD | 7:BA:165:THR:HG21 | 2.41 | 0.61 |
| 7:BA:151:LEU:HD12 | 7:BA:168:LEU:HD22 | 1.83 | 0.61 |
| 11:BF:135:ASP:OD1 | 11:BF:136:LYS:N | 2.33 | 0.61 |
| 1:BI:238:PHE:CE1 | 1:BI:262:PRO:HD2 | 2.36 | 0.61 |
| 2:C:159:ASP:HB3 | 2:C:162:SER:H | 1.65 | 0.61 |
| 2:C:59:LEU:HD13 | 2:C:67:PHE:CE2 | 2.36 | 0.61 |
| 4:CC:111:ASN:ND2 | 4:CC:116:ILE:H | 1.98 | 0.61 |
| 4:CC:193:HIS:HB3 | 4:CC:196:GLU:HG3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:72:THR:OG1 | 5:CF:101:THR:O | 2.19 | 0.61 |
| 5:CH:256:SER:O | 5:CH:258:TYR:N | 2.33 | 0.61 |
| 7:DB:2:SER:O | 7:DB:6:TYR:N | 2.25 | 0.61 |
| 7:DB:309:ALA:HB3 | 7:DD:303:GLU:HA | 1.83 | 0.61 |
| 3:E:261:ALA:O | 3:E:266:ASN:ND2 | 2.34 | 0.61 |
| 1:EA:21:PHE:CE2 | 1:EA:75:VAL:HG11 | 2.35 | 0.61 |
| 2:EC:159:ASP:HB3 | 2:EC:162:SER:H | 1.65 | 0.61 |
| 2:EC:211:VAL:N | 2:EC:220:LYS:O | 2.27 | 0.61 |
| 3:ED:43:ARG:HH22 | 3:ED:47:TRP:HB3 | 1.66 | 0.61 |
| 4:EH:111:ASN:ND2 | 4:EH:116:ILE:H | 1.98 | 0.61 |
| 5:EI:206:PHE:CZ | 5:EI:221:GLU:HG2 | 2.35 | 0.61 |
| 5:EI:399:ILE:HG23 | 5:FA:399:ILE:HD13 | 1.82 | 0.61 |
| 5:EJ:8:GLY:HA3 | 5:EJ:15:THR:HG23 | 1.83 | 0.61 |
| 7:FE:303:GLU:HA | 7:FF:309:ALA:HB3 | 1.82 | 0.61 |
| 7:FE:55:LYS:HB3 | 7:FG:57:ILE:HG22 | 1.81 | 0.61 |
| 4:G:111:ASN:ND2 | 4:G:116:ILE:H | 1.98 | 0.61 |
| 1:GE:352:ARG:HG3 | 1:GE:395:TYR:CZ | 2.36 | 0.61 |
| 2:GF:98:GLU:N | 2:GF:98:GLU:OE1 | 2.30 | 0.61 |
| 2:GF:1030:ILE:HD11 | 3:GH:7:ILE:HD11 | 1.83 | 0.61 |
| 4:GI:53:GLY:HA2 | 4:GI:59:GLN:H | 1.66 | 0.61 |
| 4:H:43:GLY:O | 4:H:68:GLN:NE2 | 2.32 | 0.61 |
| 5:HD:290:SER:CB | 5:HD:371:PHE:H | 2.14 | 0.61 |
| 5:I:290:SER:CB | 5:I:370:HIS:HA | 2.31 | 0.61 |
| 5:I:24:ILE:HG13 | 5:K:7:ILE:HD11 | 1.81 | 0.61 |
| 7:P:71:ASN:O | 7:P:73:THR:HG22 | 2.01 | 0.61 |
| 1:Y:321:ASP:OD1 | 1:Y:322:ILE:N | 2.33 | 0.61 |
| 13:YA:376[A]:PHE:CZ | 13:YB:447[A]:ASN:HB3 | 2.35 | 0.61 |
| 13:YA:437[C]:ASN:HB3 | 13:YA:439[C]:TYR:HE1 | 1.66 | 0.61 |
| 13:YA:534[B]:LEU:HD11 | 13:YA:536[B]:TRP:HE1 | 1.66 | 0.61 |
| 13:YB:313[E]:ASP:O | 13:YC:367[E]:PRO:HD3 | 2.01 | 0.61 |
| 13:YB:534[F]:LEU:HD11 | 13:YB:536[F]:TRP:HE1 | 1.66 | 0.61 |
| 13:YB:87[C]:LEU:HD21 | 13:YB:95[C]:ILE:HG23 | 1.80 | 0.61 |
| 13:YB:76[A]:PRO:HG3 | 13:YB:96[A]:VAL:HB | 1.83 | 0.61 |
| 13:YC:534[D]:LEU:HD11 | 13:YC:536[D]:TRP:HE1 | 1.66 | 0.61 |
| 13:YA:59[E]:GLN:HA | 13:YC:61[E]:ILE:CG2 | 2.27 | 0.61 |
| 13:YA:72[D]:SER:O | 13:YC:61[D]:ILE:HD11 | 2.00 | 0.61 |
| 13:YC:57[D]:VAL:HB | 13:YC:76[D]:PRO:HB3 | 1.83 | 0.61 |
| 13:YC:87[A]:LEU:HD21 | 13:YC:95[A]:ILE:HG23 | 1.80 | 0.61 |
| 14:YD:118[B]:LEU:HD23 | 14:YD:139[B]:ILE:HD13 | 1.83 | 0.61 |
| 14:YD:35[F]:ILE:HA | 14:YD:54[F]:PHE:HB3 | 1.83 | 0.61 |
| 14:YE:125[D]:PHE:CE2 | 14:YE:134[D]:GLU:HG3 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:184[B]:LYS:HE3 | 14:YE:367[B]:ILE:HG21 | 1.83 | 0.61 |
| 14:YE:294[D]:GLU:O | 14:YE:297[D]:ARG:N | 2.34 | 0.61 |
| 14:YE:294[B]:GLU:O | 14:YE:297[B]:ARG:N | 2.34 | 0.61 |
| 14:YE:312[F]:THR:OG1 | 14:YE:313[F]:ILE:N | 2.30 | 0.61 |
| 14:YF:294[F]:GLU:O | 14:YF:297[F]:ARG:N | 2.34 | 0.61 |
| 14:YF:294[E]:GLU:O | 14:YF:297[E]:ARG:N | 2.34 | 0.61 |
| 14:YF:360[A]:ASN:N | 14:YF:360[A]:ASN:HD22 | 1.98 | 0.61 |
| 2:Z:304:VAL:HG13 | 2:Z:327:ARG:NH1 | 2.16 | 0.61 |
| 5:AC:95:ALA:HB3 | 5:AC:133:LEU:HB2 | 1.83 | 0.61 |
| 5:AD:95:ALA:HB3 | 5:AD:133:LEU:HB2 | 1.82 | 0.61 |
| 7:AI:194:ALA:HB2 | 7:AI:208:TYR:HB3 | 1.81 | 0.61 |
| 7:AI:93:THR:HG22 | 7:AI:94:VAL:HG23 | 1.83 | 0.61 |
| 10:BE:42:ARG:HG3 | 10:BE:58:TYR:HB3 | 1.83 | 0.61 |
| 1:BH:242:GLU:O | 1:BH:256:TYR:OH | 2.16 | 0.61 |
| 1:A:60:LEU:HD22 | 2:C:671:TYR:CE1 | 2.36 | 0.61 |
| 3:CB:46:PRO:HA | 3:CB:270:ARG:HH21 | 1.65 | 0.61 |
| 4:CC:53:GLY:HA2 | 4:CC:59:GLN:H | 1.66 | 0.61 |
| 5:CG:153:LYS:HG2 | 5:CG:154:ILE:H | 1.64 | 0.61 |
| 5:CG:213:GLY:HA2 | 5:CG:221:GLU:HB2 | 1.83 | 0.61 |
| 5:CG:189:ASN:HD21 | 5:CH:150:GLN:NE2 | 1.98 | 0.61 |
| 7:DD:236:VAL:HG21 | 7:DD:249:THR:HB | 1.81 | 0.61 |
| 8:DE:43:ALA:O | 8:DE:162:TRP:NE1 | 2.33 | 0.61 |
| 1:EA:41:ASN:OD1 | 1:EA:42:GLU:N | 2.34 | 0.61 |
| 2:EC:150:SER:OG | 2:EC:151:PHE:N | 2.33 | 0.61 |
| 2:EC:360:ASN:C | 2:EC:362:LYS:H | 2.02 | 0.61 |
| 2:EC:506:MET:HB3 | 3:GH:176:ALA:HB1 | 1.82 | 0.61 |
| 2:EC:909:THR:OG1 | 2:EC:910:GLU:OE1 | 2.11 | 0.61 |
| 4:EF:165:GLU:HB3 | 4:EH:171:LYS:HB2 | 1.82 | 0.61 |
| 4:EG:111:ASN:ND2 | 4:EG:116:ILE:H | 1.98 | 0.61 |
| 5:EI:95:ALA:HB3 | 5:EI:133:LEU:HB2 | 1.83 | 0.61 |
| 5:EJ:262:GLN:HG2 | 5:EJ:382:ASN:HD22 | 1.66 | 0.61 |
| 6:FC:95:THR:N | 6:FC:174:TYR:O | 2.34 | 0.61 |
| 7:FG:120:LYS:O | 7:FG:124:ALA:N | 2.32 | 0.61 |
| 7:FG:453:GLU:OE2 | 7:FG:471:THR:N | 2.29 | 0.61 |
| 1:GD:96:ASN:HB3 | 1:GD:333:ARG:HB2 | 1.82 | 0.61 |
| 4:GI:43:GLY:O | 4:GI:68:GLN:NE2 | 2.32 | 0.61 |
| 4:H:53:GLY:HA2 | 4:H:59:GLN:H | 1.66 | 0.61 |
| 5:HD:174:GLN:HE21 | 5:HD:177:PHE:HE1 | 1.49 | 0.61 |
| 5:HD:89:TYR:O | 5:HD:91:LYS:N | 2.33 | 0.61 |
| 12:GC:144:ASN:H | 10:ID:58:TYR:HE1 | 1.48 | 0.61 |
| 6:L:13:ARG:HB2 | 6:N:10:VAL:HA | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:437[E]:ASN:HB3 | 13:YC:439[E]:TYR:HE1 | 1.66 | 0.61 |
| 13:YB:468[E]:ASP:HB3 | 13:YC:461[E]:SER:HA | 1.83 | 0.61 |
| 14:YD:125[F]:PHE:CE2 | 14:YD:134[F]:GLU:HG3 | 2.30 | 0.61 |
| 14:YD:294[A]:GLU:O | 14:YD:297[A]:ARG:N | 2.34 | 0.61 |
| 14:YE:118[C]:LEU:HD23 | 14:YE:139[C]:ILE:HD13 | 1.82 | 0.61 |
| 14:YE:332[A]:GLN:HB3 | 14:YF:61[A]:HIS:CE1 | 2.35 | 0.61 |
| 14:YF:184[A]:LYS:HE3 | 14:YF:367[A]:ILE:HG21 | 1.83 | 0.61 |
| 14:YF:184[F]:LYS:HE3 | 14:YF:367[F]:ILE:HG21 | 1.83 | 0.61 |
| 2:Z:575:PHE:O | 2:Z:607:THR:OG1 | 2.13 | 0.61 |
| 2:Z:59:LEU:HD13 | 2:Z:67:PHE:CE2 | 2.36 | 0.61 |
| 5:AD:146:VAL:HB | 5:AE:153:LYS:HA | 1.83 | 0.60 |
| 5:AC:407:TYR:OH | 5:AE:403:THR:HA | 2.00 | 0.60 |
| 5:AD:313:PHE:HE1 | 6:AF:8:ALA:HB1 | 1.66 | 0.60 |
| 7:AJ:211:SER:H | 7:AJ:214:THR:HG1 | 1.47 | 0.60 |
| 10:BE:236:GLU:C | 10:BE:287:VAL:HB | 2.22 | 0.60 |
| 2:C:64:ASN:OD1 | 2:C:65:ASN:N | 2.33 | 0.60 |
| 5:CF:221:GLU:OE2 | 5:CF:233:ARG:NH2 | 2.34 | 0.60 |
| 5:CG:172:GLN:HG2 | 5:CG:173:GLY:H | 1.65 | 0.60 |
| 6:CJ:95:THR:N | 6:CJ:174:TYR:O | 2.34 | 0.60 |
| 7:DD:151:LEU:HD12 | 7:DD:168:LEU:HD22 | 1.83 | 0.60 |
| 11:DI:135:ASP:CG | 11:DI:136:LYS:H | 2.02 | 0.60 |
| 4:EF:193:HIS:HB3 | 4:EF:196:GLU:HG3 | 1.83 | 0.60 |
| 4:F:193:HIS:HB3 | 4:F:196:GLU:HG3 | 1.83 | 0.60 |
| 6:FD:95:THR:N | 6:FD:174:TYR:O | 2.34 | 0.60 |
| 7:FE:140:GLY:HA2 | 7:FG:129:PHE:CZ | 2.36 | 0.60 |
| 7:FE:212:PRO:HG3 | 7:FF:199:VAL:HG12 | 1.83 | 0.60 |
| 7:FF:71:ASN:O | 7:FF:73:THR:HG22 | 2.01 | 0.60 |
| 7:FG:118:PRO:HA | 7:FG:121:PHE:HB3 | 1.81 | 0.60 |
| 4:G:53:GLY:HA2 | 4:G:59:GLN:H | 1.66 | 0.60 |
| 1:GE:455:PHE:CD1 | 1:GE:639:LEU:HD12 | 2.35 | 0.60 |
| 2:GF:92:SER:OG | 2:GF:93:ASP:N | 2.32 | 0.60 |
| 5:HB:221:GLU:OE2 | 5:HB:233:ARG:NH2 | 2.34 | 0.60 |
| 5:HC:151:ILE:HD12 | 5:HC:152:ASP:H | 1.66 | 0.60 |
| 5:I:154:ILE:HG12 | 5:J:153:LYS:HZ2 | 1.66 | 0.60 |
| 5:I:89:TYR:O | 5:I:91:LYS:N | 2.34 | 0.60 |
| 7:O:117:THR:HG23 | 7:O:120:LYS:H | 1.66 | 0.60 |
| 7:O:303:GLU:HA | 7:P:309:ALA:HB3 | 1.82 | 0.60 |
| 7:Q:310:ASN:OD1 | 7:Q:311:GLY:N | 2.31 | 0.60 |
| 10:U:129:LEU:HD11 | 10:U:225:ILE:HD11 | 1.83 | 0.60 |
| 13:YA:193[F]:ASP:OD1 | 13:YA:197[F]:TYR:N | 2.31 | 0.60 |
| 13:YA:438[E]:LEU:HD22 | 13:YC:442[E]:THR:HG21 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:534[D]:LEU:HD11 | 13:YA:536[D]:TRP:HE1 | 1.66 | 0.60 |
| 13:YB:437[B]:ASN:HB3 | 13:YB:439[B]:TYR:HE1 | 1.66 | 0.60 |
| 13:YB:468[D]:ASP:HB3 | 13:YC:461[D]:SER:HA | 1.83 | 0.60 |
| 14:YD:294[C]:GLU:O | 14:YD:297[C]:ARG:N | 2.34 | 0.60 |
| 14:YD:294[F]:GLU:O | 14:YD:297[F]:ARG:N | 2.34 | 0.60 |
| 14:YD:332[E]:GLN:HB3 | 14:YE:61[E]:HIS:CE1 | 2.36 | 0.60 |
| 14:YD:70[B]:ILE:O | 14:YD:88[B]:TYR:N | 2.34 | 0.60 |
| 14:YE:184[E]:LYS:HE3 | 14:YE:367[E]:ILE:HG21 | 1.83 | 0.60 |
| 14:YE:35[E]:ILE:HA | 14:YE:54[E]:PHE:HB3 | 1.83 | 0.60 |
| 14:YF:118[D]:LEU:HD23 | 14:YF:139[D]:ILE:HD13 | 1.83 | 0.60 |
| 14:YF:35[B]:ILE:HA | 14:YF:54[B]:PHE:HB3 | 1.83 | 0.60 |
| 14:YF:70[D]:ILE:O | 14:YF:88[D]:TYR:N | 2.34 | 0.60 |
| 5:AD:60:LEU:HG | 5:AD:79:ILE:HG22 | 1.82 | 0.60 |
| 7:AJ:163:LEU:HB3 | 7:BA:155:ASP:HA | 1.82 | 0.60 |
| 7:BA:365:GLY:HA3 | 7:BA:392:LEU:HD12 | 1.82 | 0.60 |
| 9:BD:56:ASP:OD1 | 9:BD:57:LEU:N | 2.34 | 0.60 |
| 12:BG:161:SER:HA | 12:BG:240:ASP:HA | 1.83 | 0.60 |
| 1:BH:126:PRO:HD2 | 1:BH:292:LEU:HD21 | 1.82 | 0.60 |
| 2:BJ:981:GLN:HG2 | 2:BJ:982:LEU:N | 2.16 | 0.60 |
| 2:C:304:VAL:HG13 | 2:C:327:ARG:NH1 | 2.16 | 0.60 |
| 2:C:768:TYR:OH | 2:C:814:HIS:O | 2.17 | 0.60 |
| 2:C:981:GLN:HG2 | 2:C:982:LEU:N | 2.16 | 0.60 |
| 4:CC:84:ARG:HE | 4:CE:64:THR:HA | 1.65 | 0.60 |
| 4:CD:111:ASN:ND2 | 4:CD:116:ILE:H | 1.98 | 0.60 |
| 4:CE:193:HIS:HB3 | 4:CE:196:GLU:HG3 | 1.83 | 0.60 |
| 7:DD:71:ASN:O | 7:DD:73:THR:HG22 | 2.02 | 0.60 |
| 9:DG:56:ASP:OD1 | 9:DG:57:LEU:N | 2.34 | 0.60 |
| 3:E:294:LYS:N | 3:E:297:TYR:OH | 2.32 | 0.60 |
| 1:EB:214:MET:N | 2:EC:733:ASP:OD2 | 2.34 | 0.60 |
| 2:EC:589:LYS:HB3 | 2:EC:592:GLY:O | 2.01 | 0.60 |
| 5:EI:221:GLU:OE2 | 5:EI:233:ARG:NH2 | 2.34 | 0.60 |
| 5:FA:196:ARG:NH1 | 7:FF:8:HIS:HB3 | 2.16 | 0.60 |
| 4:G:193:HIS:HB3 | 4:G:196:GLU:HG3 | 1.83 | 0.60 |
| 1:GD:378:PRO:O | 1:GD:379:LYS:HG2 | 2.02 | 0.60 |
| 1:GE:238:PHE:CE1 | 1:GE:262:PRO:HD2 | 2.36 | 0.60 |
| 2:GF:403:ILE:HG21 | 2:GF:417:PHE:HB3 | 1.84 | 0.60 |
| 2:GF:376:PHE:HZ | 2:GF:441:VAL:HG11 | 1.65 | 0.60 |
| 2:GF:59:LEU:HD13 | 2:GF:67:PHE:CE2 | 2.36 | 0.60 |
| 2:GF:950:GLU:N | 2:GF:950:GLU:OE1 | 2.24 | 0.60 |
| 2:GF:87:GLN:HE21 | 3:GG:158:GLY:HA2 | 1.66 | 0.60 |
| 3:GG:228:ASN:OD1 | 3:GG:229:LEU:N | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:114:CYS:HA | 3:GH:120:ASN:HD21 | 1.67 | 0.60 |
| 3:GH:261:ALA:O | 3:GH:266:ASN:ND2 | 2.34 | 0.60 |
| 4:F:84:ARG:HE | 4:H:64:THR:HA | 1.65 | 0.60 |
| 4:HA:42:PHE:O | 4:HA:62:HIS:ND1 | 2.27 | 0.60 |
| 5:HC:212:PHE:HZ | 5:HC:230:ILE:HB | 1.64 | 0.60 |
| 5:HC:8:GLY:HA3 | 5:HC:15:THR:HG23 | 1.83 | 0.60 |
| 6:HE:95:THR:N | 6:HE:174:TYR:O | 2.34 | 0.60 |
| 6:FB:75:THR:HB | 7:HI:167:GLN:HE22 | 1.65 | 0.60 |
| 7:HI:71:ASN:O | 7:HI:73:THR:HG22 | 2.01 | 0.60 |
| 5:I:323:THR:HG23 | 5:I:359:GLU:HB2 | 1.83 | 0.60 |
| 5:J:36:GLU:HG3 | 5:K:43:PRO:HG2 | 1.84 | 0.60 |
| 5:K:290:SER:CB | 5:K:371:PHE:H | 2.14 | 0.60 |
| 7:O:186:SER:O | 7:Q:192:GLN:NE2 | 2.34 | 0.60 |
| 1:X:332:LYS:HE3 | 1:X:348:PHE:HE1 | 1.66 | 0.60 |
| 1:X:552:LYS:HA | 1:X:594:GLU:HA | 1.83 | 0.60 |
| 1:Y:495:PRO:O | 1:Y:498:GLY:N | 2.32 | 0.60 |
| 13:YA:437[D]:ASN:HB3 | 13:YA:439[D]:TYR:HE1 | 1.67 | 0.60 |
| 13:YA:57[A]:VAL:HB | 13:YA:76[A]:PRO:HB3 | 1.83 | 0.60 |
| 13:YB:57[D]:VAL:HB | 13:YB:76[D]:PRO:HB3 | 1.83 | 0.60 |
| 13:YB:66[E]:MET:SD | 13:YC:121[E]:TYR:HB3 | 2.41 | 0.60 |
| 13:YB:313[B]:ASP:O | 13:YC:367[B]:PRO:HD3 | 2.01 | 0.60 |
| 13:YC:534[F]:LEU:HD11 | 13:YC:536[F]:TRP:HE1 | 1.66 | 0.60 |
| 14:YD:35[A]:ILE:HA | 14:YD:54[A]:PHE:HB3 | 1.83 | 0.60 |
| 14:YD:184[B]:LYS:HE3 | 14:YD:367[B]:ILE:HG21 | 1.83 | 0.60 |
| 14:YD:66[E]:GLY:N | 14:YD:68[E]:GLU:OE2 | 2.33 | 0.60 |
| 14:YD:70[E]:ILE:O | 14:YD:88[E]:TYR:N | 2.34 | 0.60 |
| 14:YE:41[D]:ARG:HG2 | 14:YE:343[D]:ILE:HG12 | 1.83 | 0.60 |
| 14:YE:35[D]:ILE:HA | 14:YE:54[D]:PHE:HB3 | 1.83 | 0.60 |
| 14:YF:294[A]:GLU:O | 14:YF:297[A]:ARG:N | 2.34 | 0.60 |
| 14:YF:294[B]:GLU:O | 14:YF:297[B]:ARG:N | 2.34 | 0.60 |
| 14:YF:35[C]:ILE:HA | 14:YF:54[C]:PHE:HB3 | 1.83 | 0.60 |
| 14:YE:332[D]:GLN:HB3 | 14:YF:61[D]:HIS:CE1 | 2.36 | 0.60 |
| 14:YF:70[F]:ILE:O | 14:YF:88[F]:TYR:N | 2.34 | 0.60 |
| 1:A:229:THR:OG1 | 1:A:231:ASP:OD1 | 2.19 | 0.60 |
| 5:AC:221:GLU:OE2 | 5:AC:233:ARG:NH2 | 2.34 | 0.60 |
| 5:AC:323:THR:HG23 | 5:AC:359:GLU:HB2 | 1.83 | 0.60 |
| 5:AD:260:ARG:O | 5:AD:261:ARG:NH1 | 2.33 | 0.60 |
| 5:AE:144:GLU:N | 5:AE:144:GLU:OE1 | 2.33 | 0.60 |
| 7:AI:186:SER:O | 7:BA:192:GLN:NE2 | 2.34 | 0.60 |
| 7:BA:118:PRO:HA | 7:BA:121:PHE:HB3 | 1.82 | 0.60 |
| 8:BC:43:ALA:O | 8:BC:162:TRP:NE1 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:332:LYS:HE3 | 1:BH:348:PHE:HE1 | 1.66 | 0.60 |
| 1:BI:496:GLU:HG3 | 2:BJ:856:ASN:O | 2.01 | 0.60 |
| 2:BJ:909:THR:OG1 | 2:BJ:910:GLU:OE1 | 2.11 | 0.60 |
| 5:CF:361:ASP:H | 5:CF:366:PRO:HA | 1.66 | 0.60 |
| 5:CG:95:ALA:HB3 | 5:CG:133:LEU:HB2 | 1.82 | 0.60 |
| 3:D:75:MET:HG2 | 3:D:299:PRO:HG3 | 1.84 | 0.60 |
| 3:E:114:CYS:HA | 3:E:120:ASN:HD21 | 1.67 | 0.60 |
| 1:EA:411:PRO:HG2 | 1:EA:413:TYR:CD2 | 2.37 | 0.60 |
| 5:EJ:213:GLY:HA2 | 5:EJ:221:GLU:HB2 | 1.83 | 0.60 |
| 5:EJ:285:LEU:HD11 | 5:EJ:375:PHE:CB | 2.28 | 0.60 |
| 5:EJ:316:ILE:HG23 | 5:FA:315:GLY:HA3 | 1.82 | 0.60 |
| 5:FA:330:HIS:ND1 | 5:FA:355:ASP:HB2 | 2.14 | 0.60 |
| 7:FE:220:SER:OG | 7:FE:226:GLY:O | 2.20 | 0.60 |
| 7:FG:2:SER:N | 7:FG:5:THR:HG1 | 2.00 | 0.60 |
| 1:GD:227:ARG:HD3 | 1:GD:237:TYR:CE2 | 2.36 | 0.60 |
| 1:GE:87:SER:OG | 1:GE:230:ILE:O | 2.12 | 0.60 |
| 2:GF:292:GLU:OE1 | 2:GF:292:GLU:N | 2.34 | 0.60 |
| 2:GF:901:ASN:OD1 | 3:GH:333:THR:OG1 | 2.19 | 0.60 |
| 7:HH:310:ASN:HA | 7:HI:316:THR:HB | 1.82 | 0.60 |
| 5:I:3:GLN:HG2 | 5:I:25:LYS:HG3 | 1.82 | 0.60 |
| 5:J:194:LYS:HB2 | 5:J:243:GLN:HB2 | 1.82 | 0.60 |
| 5:J:63:GLU:HB2 | 5:J:68:TYR:OH | 2.00 | 0.60 |
| 5:K:419:ASP:OD1 | 5:K:420:VAL:N | 2.34 | 0.60 |
| 1:Y:352:ARG:HG3 | 1:Y:395:TYR:CZ | 2.36 | 0.60 |
| 13:YA:376[C]:PHE:CZ | 13:YB:447[C]:ASN:HB3 | 2.35 | 0.60 |
| 13:YB:534[B]:LEU:HD11 | 13:YB:536[B]:TRP:HE1 | 1.66 | 0.60 |
| 13:YB:66[B]:MET:SD | 13:YC:121[B]:TYR:HB3 | 2.41 | 0.60 |
| 13:YB:7[D]:ASN:ND2 | 13:YC:9[D]:ASN:HA | 2.14 | 0.60 |
| 14:YD:184[C]:LYS:HE3 | 14:YD:367[C]:ILE:HG21 | 1.83 | 0.60 |
| 14:YD:184[D]:LYS:HE3 | 14:YD:367[D]:ILE:HG21 | 1.83 | 0.60 |
| 14:YD:184[E]:LYS:HE3 | 14:YD:367[E]:ILE:HG21 | 1.84 | 0.60 |
| 14:YD:35[E]:ILE:HA | 14:YD:54[E]:PHE:HB3 | 1.83 | 0.60 |
| 14:YE:184[F]:LYS:HE3 | 14:YE:367[F]:ILE:HG21 | 1.83 | 0.60 |
| 14:YF:118[A]:LEU:HD23 | 14:YF:139[A]:ILE:HD13 | 1.83 | 0.60 |
| 14:YF:184[D]:LYS:HE3 | 14:YF:367[D]:ILE:HG21 | 1.83 | 0.60 |
| 2:Z:150:SER:OG | 2:Z:151:PHE:N | 2.33 | 0.60 |
| 1:A:278:ALA:HB2 | 1:A:317:GLY:H | 1.67 | 0.60 |
| 6:AF:77:VAL:HG23 | 7:DC:167:GLN:NE2 | 2.16 | 0.60 |
| 5:AC:356:TYR:HE1 | 6:AH:4:LEU:HD13 | 1.66 | 0.60 |
| 7:AJ:71:ASN:O | 7:AJ:73:THR:HG22 | 2.01 | 0.60 |
| 7:AI:260:ARG:NH1 | 7:BA:251:ASN:O | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BA:296:ILE:HG22 | 7:BA:298:GLY:H | 1.67 | 0.60 |
| 7:BA:71:ASN:O | 7:BA:73:THR:HG22 | 2.02 | 0.60 |
| 1:BH:227:ARG:HD3 | 1:BH:237:TYR:CE2 | 2.36 | 0.60 |
| 1:BI:448:TYR:HA | 1:BI:452:VAL:HG12 | 1.83 | 0.60 |
| 2:BJ:150:SER:OG | 2:BJ:151:PHE:N | 2.33 | 0.60 |
| 2:BJ:239:TYR:HB3 | 2:BJ:313:CYS:SG | 2.41 | 0.60 |
| 2:BJ:403:ILE:HG21 | 2:BJ:417:PHE:HB3 | 1.84 | 0.60 |
| 2:C:364:VAL:HG11 | 2:C:390:PRO:HB3 | 1.82 | 0.60 |
| 3:CB:261:ALA:O | 3:CB:266:ASN:ND2 | 2.34 | 0.60 |
| 5:CF:24:ILE:HG13 | 5:CH:7:ILE:HD11 | 1.82 | 0.60 |
| 5:CG:285:LEU:HD11 | 5:CG:375:PHE:CB | 2.28 | 0.60 |
| 5:CH:419:ASP:OD1 | 5:CH:420:VAL:N | 2.34 | 0.60 |
| 3:D:43:ARG:HH22 | 3:D:47:TRP:HB3 | 1.66 | 0.60 |
| 6:CI:11:ILE:HA | 6:DA:7:LYS:HD3 | 1.82 | 0.60 |
| 7:DB:96:GLY:N | 7:DD:97:LEU:HB3 | 2.17 | 0.60 |
| 10:DH:236:GLU:C | 10:DH:287:VAL:HB | 2.22 | 0.60 |
| 2:EC:316:ASP:HB3 | 2:EC:330:LYS:HE2 | 1.84 | 0.60 |
| 4:EH:43:GLY:O | 4:EH:68:GLN:NE2 | 2.32 | 0.60 |
| 5:FA:174:GLN:HE21 | 5:FA:177:PHE:HE1 | 1.49 | 0.60 |
| 7:FG:365:GLY:HA3 | 7:FG:392:LEU:HD12 | 1.83 | 0.60 |
| 1:GD:552:LYS:HA | 1:GD:594:GLU:HA | 1.83 | 0.60 |
| 1:GE:448:TYR:HA | 1:GE:452:VAL:HG12 | 1.83 | 0.60 |
| 2:GF:768:TYR:OH | 2:GF:814:HIS:O | 2.17 | 0.60 |
| 4:H:193:HIS:HB3 | 4:H:196:GLU:HG3 | 1.83 | 0.60 |
| 5:HC:103:ASN:N | 5:HC:127:ASN:O | 2.31 | 0.60 |
| 5:HC:262:GLN:HG2 | 5:HC:382:ASN:HD22 | 1.66 | 0.60 |
| 5:HC:312:ARG:O | 5:HC:382:ASN:N | 2.30 | 0.60 |
| 5:HD:86:VAL:HG22 | 5:HD:87:ASN:H | 1.67 | 0.60 |
| 5:HC:139:ALA:HB3 | 5:HD:99:PHE:HB3 | 1.84 | 0.60 |
| 7:HJ:453:GLU:OE2 | 7:HJ:471:THR:N | 2.29 | 0.60 |
| 5:I:72:THR:OG1 | 5:I:101:THR:O | 2.19 | 0.60 |
| 5:I:196:ARG:NH2 | 5:K:199:GLU:OE1 | 2.34 | 0.60 |
| 9:IC:100:ASP:OD1 | 9:IC:101:ASP:N | 2.34 | 0.60 |
| 7:P:196:VAL:HG11 | 6:HE:140:PHE:CZ | 2.36 | 0.60 |
| 7:Q:100:TYR:CD1 | 7:Q:115:SER:HB2 | 2.37 | 0.60 |
| 8:S:76:ASP:OD1 | 8:S:77:GLU:N | 2.35 | 0.60 |
| 1:X:227:ARG:HD3 | 1:X:237:TYR:CE2 | 2.36 | 0.60 |
| 13:YA:534[E]:LEU:HD11 | 13:YA:536[E]:TRP:HE1 | 1.66 | 0.60 |
| 13:YB:437[A]:ASN:HB3 | 13:YB:439[A]:TYR:HE1 | 1.67 | 0.60 |
| 13:YA:554[F]:MET:HE2 | 13:YB:550[F]:TRP:CD1 | 2.36 | 0.60 |
| 13:YB:66[A]:MET:SD | 13:YC:121[A]:TYR:HB3 | 2.41 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:567[F]:ILE:O | 13:YC:575[F]:GLY:N | 2.34 | 0.60 |
| 11:BF:178:ASN:N | 14:YE:217[A]:SER:O | 2.32 | 0.60 |
| 14:YE:294[A]:GLU:O | 14:YE:297[A]:ARG:N | 2.34 | 0.60 |
| 14:YE:70[E]:ILE:O | 14:YE:88[E]:TYR:N | 2.34 | 0.60 |
| 14:YF:118[E]:LEU:HD23 | 14:YF:139[E]:ILE:HD13 | 1.84 | 0.60 |
| 14:YF:70[A]:ILE:O | 14:YF:88[A]:TYR:N | 2.34 | 0.60 |
| 2:Z:376:PHE:HZ | 2:Z:441:VAL:HG11 | 1.65 | 0.60 |
| 2:Z:378:LEU:HD23 | 2:Z:434:MET:HB2 | 1.84 | 0.60 |
| 4:AB:42:PHE:O | 4:AB:62:HIS:ND1 | 2.27 | 0.60 |
| 5:AC:569:TYR:H | 5:AD:550:VAL:HB | 1.67 | 0.60 |
| 6:AF:75:THR:HB | 7:DC:167:GLN:NE2 | 2.16 | 0.60 |
| 7:AI:192:GLN:NE2 | 7:AJ:186:SER:O | 2.35 | 0.60 |
| 7:AI:134:SER:HB2 | 7:BA:143:LYS:HA | 1.84 | 0.60 |
| 2:BJ:145:ALA:HB2 | 2:BJ:542:THR:HB | 1.83 | 0.60 |
| 2:BJ:92:SER:OG | 2:BJ:93:ASP:N | 2.32 | 0.60 |
| 2:C:514:PHE:HB3 | 2:C:523:ARG:HB3 | 1.82 | 0.60 |
| 2:BJ:87:GLN:HE21 | 3:CA:158:GLY:HA2 | 1.66 | 0.60 |
| 3:CA:43:ARG:NH2 | 3:CA:47:TRP:HB3 | 2.15 | 0.60 |
| 5:CF:3:GLN:HG2 | 5:CF:25:LYS:HG3 | 1.82 | 0.60 |
| 5:CH:313:PHE:HE1 | 6:CJ:8:ALA:HB1 | 1.65 | 0.60 |
| 7:DD:7:GLN:HB3 | 7:DD:15:TYR:CZ | 2.36 | 0.60 |
| 10:DH:42:ARG:HG3 | 10:DH:58:TYR:HB3 | 1.83 | 0.60 |
| 3:E:46:PRO:HA | 3:E:270:ARG:HH21 | 1.66 | 0.60 |
| 1:EA:229:THR:OG1 | 1:EA:231:ASP:OD1 | 2.19 | 0.60 |
| 1:EB:539:ARG:H | 1:EB:556:GLY:HA3 | 1.67 | 0.60 |
| 2:EC:185:LYS:HE3 | 2:EC:189:ARG:CZ | 2.32 | 0.60 |
| 2:EC:376:PHE:HZ | 2:EC:441:VAL:HG11 | 1.65 | 0.60 |
| 5:EJ:78:THR:HA | 5:EJ:108:THR:HB | 1.84 | 0.60 |
| 4:F:131:LYS:N | 4:F:160:TRP:O | 2.29 | 0.60 |
| 5:FA:213:GLY:O | 5:FA:214:SER:OG | 2.19 | 0.60 |
| 5:FA:290:SER:CB | 5:FA:371:PHE:H | 2.14 | 0.60 |
| 1:GD:17:ILE:HG22 | 1:GD:19:GLU:H | 1.67 | 0.60 |
| 1:GD:231:ASP:OD1 | 1:GD:232:GLY:N | 2.35 | 0.60 |
| 1:GD:411:PRO:HG2 | 1:GD:413:TYR:CD2 | 2.37 | 0.60 |
| 2:GF:143:MET:HG2 | 2:GF:544:VAL:HG13 | 1.83 | 0.60 |
| 2:GF:149:GLU:O | 2:GF:150:SER:OG | 2.18 | 0.60 |
| 2:GF:239:TYR:HB3 | 2:GF:313:CYS:SG | 2.41 | 0.60 |
| 2:GF:333:ASN:HB2 | 4:GI:17:ASN:O | 2.01 | 0.60 |
| 3:GG:54:VAL:HG23 | 3:GH:5:SER:HA | 1.82 | 0.60 |
| 4:GI:111:ASN:ND2 | 4:GI:116:ILE:H | 1.98 | 0.60 |
| 4:GJ:171:LYS:HB2 | 4:HA:165:GLU:HB3 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:89:TYR:O | 5:HB:91:LYS:N | 2.34 | 0.60 |
| 5:HC:78:THR:HA | 5:HC:108:THR:HB | 1.84 | 0.60 |
| 7:HH:47:VAL:HA | 7:HH:57:ILE:HD12 | 1.83 | 0.60 |
| 7:HH:441:GLN:NE2 | 7:HJ:509:GLY:HA3 | 2.12 | 0.60 |
| 5:I:221:GLU:OE2 | 5:I:233:ARG:NH2 | 2.34 | 0.60 |
| 5:I:184:THR:H | 5:I:307:ASN:HD22 | 1.47 | 0.60 |
| 5:I:71:ASN:OD1 | 5:I:73:SER:N | 2.27 | 0.60 |
| 8:IA:76:ASP:OD1 | 8:IA:77:GLU:N | 2.35 | 0.60 |
| 7:O:260:ARG:NH1 | 7:Q:251:ASN:O | 2.34 | 0.60 |
| 7:O:441:GLN:NE2 | 7:Q:509:GLY:HA3 | 2.13 | 0.60 |
| 7:P:163:LEU:HB3 | 7:Q:155:ASP:HA | 1.82 | 0.60 |
| 7:Q:71:ASN:O | 7:Q:73:THR:HG22 | 2.02 | 0.60 |
| 13:YA:567[E]:ILE:O | 13:YC:575[E]:GLY:N | 2.34 | 0.60 |
| 13:YA:57[D]:VAL:HB | 13:YA:76[D]:PRO:HB3 | 1.83 | 0.60 |
| 13:YB:534[C]:LEU:HD11 | 13:YB:536[C]:TRP:HE1 | 1.66 | 0.60 |
| 13:YB:65[A]:ALA:N | 13:YB:69[A]:ILE:O | 2.35 | 0.60 |
| 13:YB:7[C]:ASN:ND2 | 13:YC:9[C]:ASN:HA | 2.14 | 0.60 |
| 11:GB:190:LYS:HE3 | 14:YD:24[F]:SER:O | 2.01 | 0.60 |
| 14:YD:41[F]:ARG:HG2 | 14:YD:343[F]:ILE:HG12 | 1.84 | 0.60 |
| 14:YD:70[D]:ILE:O | 14:YD:88[D]:TYR:N | 2.34 | 0.60 |
| 13:YB:47[F]:ILE:HG23 | 14:YE:123[F]:PRO:CG | 2.30 | 0.60 |
| 14:YE:184[A]:LYS:HE3 | 14:YE:367[A]:ILE:HG21 | 1.83 | 0.60 |
| 14:YE:70[B]:ILE:O | 14:YE:88[B]:TYR:N | 2.34 | 0.60 |
| 14:YE:70[C]:ILE:O | 14:YE:88[C]:TYR:N | 2.34 | 0.60 |
| 14:YF:118[F]:LEU:HD23 | 14:YF:139[F]:ILE:HD13 | 1.84 | 0.60 |
| 14:YF:41[B]:ARG:HG2 | 14:YF:343[B]:ILE:HG12 | 1.84 | 0.60 |
| 14:YF:184[B]:LYS:HE3 | 14:YF:367[B]:ILE:HG21 | 1.83 | 0.60 |
| 2:Z:239:TYR:HB3 | 2:Z:313:CYS:SG | 2.41 | 0.60 |
| 1:A:553:VAL:N | 1:A:593:GLY:O | 2.21 | 0.60 |
| 5:AC:557:TYR:OH | 5:AD:556:GLN:OE1 | 2.20 | 0.60 |
| 5:AE:213:GLY:O | 5:AE:214:SER:OG | 2.19 | 0.60 |
| 7:AI:117:THR:HG23 | 7:AI:120:LYS:H | 1.66 | 0.60 |
| 8:BC:23:VAL:HB | 8:BC:113:VAL:HG23 | 1.84 | 0.60 |
| 10:BE:129:LEU:HD11 | 10:BE:225:ILE:HD11 | 1.83 | 0.60 |
| 1:BI:281:ASN:HA | 1:BI:313:ALA:HB3 | 1.84 | 0.60 |
| 1:BI:539:ARG:H | 1:BI:556:GLY:HA3 | 1.67 | 0.60 |
| 2:BJ:304:VAL:HG13 | 2:BJ:327:ARG:NH1 | 2.16 | 0.60 |
| 7:DB:47:VAL:HA | 7:DB:57:ILE:HD12 | 1.83 | 0.60 |
| 7:DC:481:SER:OG | 7:DD:449:GLY:O | 2.18 | 0.60 |
| 7:DD:2:SER:N | 7:DD:5:THR:HG1 | 2.00 | 0.60 |
| 8:BB:125:LYS:HG2 | 8:DE:79:HIS:HB2 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:DG:104:LEU:O | 9:DG:126:LEU:N | 2.31 | 0.60 |
| 1:EA:126:PRO:HD2 | 1:EA:292:LEU:HD21 | 1.82 | 0.60 |
| 1:EA:552:LYS:HA | 1:EA:594:GLU:HA | 1.83 | 0.60 |
| 1:EB:448:TYR:HA | 1:EB:452:VAL:HG12 | 1.83 | 0.60 |
| 2:EC:143:MET:HG2 | 2:EC:544:VAL:HG13 | 1.83 | 0.60 |
| 2:EC:703:TYR:O | 2:EC:706:SER:N | 2.31 | 0.60 |
| 3:EE:261:ALA:O | 3:EE:266:ASN:ND2 | 2.34 | 0.60 |
| 5:EI:223:VAL:HB | 5:EI:224:PRO:HD3 | 1.83 | 0.60 |
| 5:EI:361:ASP:H | 5:EI:366:PRO:HA | 1.66 | 0.60 |
| 5:EJ:600:ARG:NE | 5:EJ:602:ALA:O | 2.32 | 0.60 |
| 4:F:111:ASN:ND2 | 4:F:116:ILE:H | 1.98 | 0.60 |
| 10:GA:236:GLU:C | 10:GA:287:VAL:HB | 2.22 | 0.60 |
| 10:GA:42:ARG:HG3 | 10:GA:58:TYR:HB3 | 1.83 | 0.60 |
| 2:GF:159:ASP:HB3 | 2:GF:162:SER:H | 1.65 | 0.60 |
| 2:GF:589:LYS:HB3 | 2:GF:592:GLY:O | 2.01 | 0.60 |
| 5:HB:3:GLN:HG2 | 5:HB:25:LYS:HG3 | 1.82 | 0.60 |
| 5:HD:196:ARG:NH1 | 7:HI:8:HIS:HB3 | 2.16 | 0.60 |
| 7:HH:117:THR:HG23 | 7:HH:120:LYS:H | 1.66 | 0.60 |
| 7:HH:260:ARG:NH1 | 7:HJ:251:ASN:O | 2.35 | 0.60 |
| 7:HJ:27:PRO:HA | 7:HJ:29:ILE:HD11 | 1.82 | 0.60 |
| 7:HJ:365:GLY:HA3 | 7:HJ:392:LEU:HD12 | 1.82 | 0.60 |
| 7:O:220:SER:OG | 7:O:226:GLY:O | 2.20 | 0.60 |
| 7:Q:151:LEU:HD12 | 7:Q:168:LEU:HD22 | 1.83 | 0.60 |
| 9:T:56:ASP:OD1 | 9:T:57:LEU:N | 2.34 | 0.60 |
| 10:U:222:ILE:O | 10:U:225:ILE:N | 2.35 | 0.60 |
| 13:YA:72[C]:SER:O | 13:YC:61[C]:ILE:HD11 | 2.01 | 0.60 |
| 13:YB:437[C]:ASN:HB3 | 13:YB:439[C]:TYR:HE1 | 1.66 | 0.60 |
| 14:YD:184[F]:LYS:HE3 | 14:YD:367[F]:ILE:HG21 | 1.83 | 0.60 |
| 14:YD:41[D]:ARG:HG2 | 14:YD:343[D]:ILE:HG12 | 1.83 | 0.60 |
| 11:GB:178:ASN:N | 14:YF:217[A]:SER:O | 2.33 | 0.60 |
| 2:Z:316:ASP:HB3 | 2:Z:330:LYS:HE2 | 1.84 | 0.60 |
| 2:Z:775:ASP:O | 2:Z:776:SER:OG | 2.20 | 0.60 |
| 1:A:378:PRO:O | 1:A:379:LYS:HG2 | 2.02 | 0.60 |
| 1:A:41:ASN:OD1 | 1:A:42:GLU:N | 2.34 | 0.60 |
| 4:AB:43:GLY:O | 4:AB:68:GLN:NE2 | 2.32 | 0.60 |
| 5:AC:459:ILE:HD11 | 5:AE:463:ALA:HB2 | 1.83 | 0.60 |
| 5:AD:20:ARG:HH12 | 5:AD:24:ILE:HD12 | 1.67 | 0.60 |
| 5:AC:279:SER:HB2 | 5:AE:326:MET:HE3 | 1.82 | 0.60 |
| 5:AE:419:ASP:OD1 | 5:AE:420:VAL:N | 2.34 | 0.60 |
| 7:AI:218:SER:O | 7:AI:227:VAL:HG22 | 2.02 | 0.60 |
| 1:BH:60:LEU:HD22 | 2:BJ:671:TYR:CE1 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:352:ARG:HG3 | 1:BI:395:TYR:CZ | 2.36 | 0.60 |
| 2:BJ:185:LYS:HE3 | 2:BJ:189:ARG:CZ | 2.31 | 0.60 |
| 2:BJ:378:LEU:HD23 | 2:BJ:434:MET:HB2 | 1.84 | 0.60 |
| 2:BJ:467:LEU:HD11 | 3:ED:56:PHE:H | 1.66 | 0.60 |
| 2:C:143:MET:HG2 | 2:C:544:VAL:HG13 | 1.83 | 0.60 |
| 5:CF:323:THR:HG23 | 5:CF:359:GLU:HB2 | 1.83 | 0.60 |
| 5:CG:20:ARG:HH12 | 5:CG:24:ILE:HD12 | 1.67 | 0.60 |
| 5:CG:78:THR:HA | 5:CG:108:THR:HB | 1.84 | 0.60 |
| 7:DB:29:ILE:HG22 | 7:DB:30:THR:N | 2.14 | 0.60 |
| 7:DC:147:LEU:HB2 | 7:DC:148:PRO:HD3 | 1.84 | 0.60 |
| 7:DD:12:GLU:HB3 | 7:DD:15:TYR:HB3 | 1.84 | 0.60 |
| 7:DC:36:ILE:HG21 | 7:DD:18:PHE:CZ | 2.36 | 0.60 |
| 7:DB:24:ASN:ND2 | 7:DD:41:PRO:HA | 2.05 | 0.60 |
| 1:EA:242:GLU:O | 1:EA:256:TYR:OH | 2.16 | 0.60 |
| 1:EB:209:TRP:O | 1:EB:212:LYS:N | 2.35 | 0.60 |
| 2:EC:239:TYR:HB3 | 2:EC:313:CYS:SG | 2.41 | 0.60 |
| 2:EC:364:VAL:HG11 | 2:EC:390:PRO:HB3 | 1.82 | 0.60 |
| 4:EH:53:GLY:HA2 | 4:EH:59:GLN:H | 1.66 | 0.60 |
| 7:FE:326:ILE:HG23 | 7:FG:323:GLY:HA2 | 1.83 | 0.60 |
| 8:FI:76:ASP:OD1 | 8:FI:77:GLU:N | 2.35 | 0.60 |
| 4:G:106:CYS:SG | 4:G:149:ARG:NH2 | 2.67 | 0.60 |
| 1:GE:539:ARG:H | 1:GE:556:GLY:HA3 | 1.67 | 0.60 |
| 5:HB:290:SER:CB | 5:HB:370:HIS:HA | 2.31 | 0.60 |
| 5:HC:60:LEU:HG | 5:HC:79:ILE:HG22 | 1.82 | 0.60 |
| 5:HD:213:GLY:O | 5:HD:214:SER:OG | 2.19 | 0.60 |
| 5:HD:419:ASP:OD1 | 5:HD:420:VAL:N | 2.34 | 0.60 |
| 7:HH:184:THR:OG1 | 7:HH:187:ASP:N | 2.34 | 0.60 |
| 7:HH:473:LYS:HB3 | 7:HI:473:LYS:HD2 | 1.84 | 0.60 |
| 7:HI:36:ILE:HG21 | 7:HJ:18:PHE:CZ | 2.36 | 0.60 |
| 7:HH:160:MET:SD | 7:HJ:165:THR:HG21 | 2.41 | 0.60 |
| 7:HI:99:ARG:HD2 | 7:HJ:95:TYR:HE1 | 1.67 | 0.60 |
| 9:IC:56:ASP:OD1 | 9:IC:57:LEU:N | 2.34 | 0.60 |
| 13:YA:437[E]:ASN:HB3 | 13:YA:439[E]:TYR:HE1 | 1.66 | 0.60 |
| 13:YB:437[F]:ASN:HB3 | 13:YB:439[F]:TYR:HE1 | 1.66 | 0.60 |
| 13:YA:558[E]:SER:HB3 | 13:YB:551[E]:THR:HG22 | 1.84 | 0.60 |
| 13:YB:291[C]:LYS:HZ3 | 13:YC:362[C]:ASP:N | 2.00 | 0.60 |
| 13:YC:534[A]:LEU:HD11 | 13:YC:536[A]:TRP:HE1 | 1.66 | 0.60 |
| 14:YD:41[C]:ARG:HG2 | 14:YD:343[C]:ILE:HG12 | 1.84 | 0.60 |
| 14:YD:70[A]:ILE:O | 14:YD:88[A]:TYR:N | 2.34 | 0.60 |
| 14:YE:35[C]:ILE:HA | 14:YE:54[C]:PHE:HB3 | 1.83 | 0.60 |
| 14:YE:35[F]:ILE:HA | 14:YE:54[F]:PHE:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:118[C]:LEU:HD23 | 14:YF:139[C]:ILE:HD13 | 1.82 | 0.60 |
| 14:YF:184[E]:LYS:HE3 | 14:YF:367[E]:ILE:HG21 | 1.83 | 0.60 |
| 14:YF:41[E]:ARG:HG2 | 14:YF:343[E]:ILE:HG12 | 1.84 | 0.60 |
| 14:YF:35[A]:ILE:HA | 14:YF:54[A]:PHE:HB3 | 1.83 | 0.60 |
| 2:Z:950:GLU:N | 2:Z:950:GLU:OE1 | 2.24 | 0.60 |
| 5:AC:361:ASP:H | 5:AC:366:PRO:HA | 1.66 | 0.60 |
| 5:AC:72:THR:OG1 | 5:AC:101:THR:O | 2.19 | 0.60 |
| 5:AD:8:GLY:HA3 | 5:AD:15:THR:HG23 | 1.83 | 0.60 |
| 8:BB:23:VAL:HB | 8:BB:113:VAL:HG23 | 1.84 | 0.60 |
| 1:BH:411:PRO:HG2 | 1:BH:413:TYR:CD2 | 2.37 | 0.60 |
| 1:BH:526:PRO:HB3 | 13:YA:254[F]:ARG:HD3 | 1.84 | 0.60 |
| 2:C:378:LEU:HD23 | 2:C:434:MET:HB2 | 1.84 | 0.60 |
| 3:CA:135:ASP:OD1 | 3:CA:136:VAL:N | 2.34 | 0.60 |
| 3:CB:114:CYS:HA | 3:CB:120:ASN:HD21 | 1.66 | 0.60 |
| 4:CE:53:GLY:HA2 | 4:CE:59:GLN:H | 1.66 | 0.60 |
| 5:CF:290:SER:CB | 5:CF:370:HIS:HA | 2.31 | 0.60 |
| 5:CF:557:TYR:OH | 5:CG:556:GLN:OE1 | 2.20 | 0.60 |
| 2:BJ:921:TRP:NE1 | 5:CG:19:LEU:HA | 2.17 | 0.60 |
| 5:CF:279:SER:HB2 | 5:CH:326:MET:HE3 | 1.82 | 0.60 |
| 7:DB:117:THR:HG23 | 7:DB:120:LYS:H | 1.67 | 0.60 |
| 7:DB:218:SER:O | 7:DB:227:VAL:HG22 | 2.02 | 0.60 |
| 1:EB:352:ARG:HG3 | 1:EB:395:TYR:CZ | 2.36 | 0.60 |
| 2:EC:92:SER:OG | 2:EC:93:ASP:N | 2.32 | 0.60 |
| 3:ED:170:PRO:HG3 | 3:ED:188:TRP:CG | 2.37 | 0.60 |
| 3:EE:46:PRO:HA | 3:EE:270:ARG:HH21 | 1.65 | 0.60 |
| 2:EC:1030:ILE:HD11 | 3:EE:7:ILE:HD11 | 1.84 | 0.60 |
| 7:FE:218:SER:O | 7:FE:227:VAL:HG22 | 2.02 | 0.60 |
| 6:CI:218:THR:HB | 7:FF:205:ARG:HH12 | 1.66 | 0.60 |
| 2:EC:654:PRO:HG3 | 9:FJ:47:ARG:HD2 | 1.83 | 0.60 |
| 2:GF:145:ALA:HB2 | 2:GF:542:THR:HB | 1.83 | 0.60 |
| 2:GF:316:ASP:HB3 | 2:GF:330:LYS:HE2 | 1.84 | 0.60 |
| 3:GG:170:PRO:HG3 | 3:GG:188:TRP:CG | 2.37 | 0.60 |
| 4:GI:131:LYS:N | 4:GI:160:TRP:O | 2.29 | 0.60 |
| 5:HB:184:THR:H | 5:HB:307:ASN:HD22 | 1.48 | 0.60 |
| 5:HC:293:PHE:HD1 | 5:HC:298:LEU:HD11 | 1.65 | 0.60 |
| 10:ID:129:LEU:HD11 | 10:ID:225:ILE:HD11 | 1.83 | 0.60 |
| 5:J:78:THR:HA | 5:J:108:THR:HB | 1.84 | 0.60 |
| 7:O:399:PHE:CD2 | 7:Q:514:PRO:HG2 | 2.36 | 0.60 |
| 7:O:422:LYS:HB3 | 7:P:504:ARG:HA | 1.84 | 0.60 |
| 7:O:192:GLN:NE2 | 7:P:186:SER:O | 2.35 | 0.60 |
| 7:Q:476:ASP:OD1 | 7:Q:479:ASN:ND2 | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:286:PHE:HB2 | 1:X:300:ILE:HD11 | 1.84 | 0.60 |
| 13:YA:193[A]:ASP:OD1 | 13:YA:197[A]:TYR:N | 2.33 | 0.60 |
| 13:YA:50[A]:GLU:OE2 | 13:YA:50[A]:GLU:N | 2.33 | 0.60 |
| 13:YA:76[D]:PRO:HG3 | 13:YA:96[D]:VAL:HB | 1.83 | 0.60 |
| 13:YA:558[D]:SER:HB3 | 13:YB:551[D]:THR:HG22 | 1.84 | 0.60 |
| 13:YB:468[B]:ASP:HB3 | 13:YC:461[B]:SER:HA | 1.83 | 0.60 |
| 14:YE:118[F]:LEU:HD23 | 14:YE:139[F]:ILE:HD13 | 1.84 | 0.60 |
| 13:YB:47[C]:ILE:HG12 | 14:YE:123[C]:PRO:HD3 | 1.83 | 0.60 |
| 14:YF:118[B]:LEU:HD23 | 14:YF:139[B]:ILE:HD13 | 1.83 | 0.60 |
| 14:YF:294[D]:GLU:O | 14:YF:297[D]:ARG:N | 2.34 | 0.60 |
| 14:YF:41[F]:ARG:HG2 | 14:YF:343[F]:ILE:HG12 | 1.84 | 0.60 |
| 14:YF:41[D]:ARG:HG2 | 14:YF:343[D]:ILE:HG12 | 1.83 | 0.60 |
| 14:YF:35[D]:ILE:HA | 14:YF:54[D]:PHE:HB3 | 1.83 | 0.60 |
| 2:Z:143:MET:HG2 | 2:Z:544:VAL:HG13 | 1.82 | 0.60 |
| 4:AB:53:GLY:HA2 | 4:AB:59:GLN:H | 1.66 | 0.60 |
| 5:AD:262:GLN:HG2 | 5:AD:382:ASN:HD22 | 1.66 | 0.60 |
| 5:AE:331:CYS:HA | 5:AE:349:TRP:HZ2 | 1.67 | 0.60 |
| 7:AI:29:ILE:HG22 | 7:AI:30:THR:N | 2.14 | 0.60 |
| 1:B:539:ARG:H | 1:B:556:GLY:HA3 | 1.67 | 0.60 |
| 7:BA:12:GLU:HB3 | 7:BA:15:TYR:HB3 | 1.84 | 0.60 |
| 7:BA:7:GLN:HB3 | 7:BA:15:TYR:CZ | 2.36 | 0.60 |
| 5:AC:234:GLN:NE2 | 7:BA:9:VAL:HG21 | 2.16 | 0.60 |
| 1:BH:17:ILE:HG22 | 1:BH:19:GLU:H | 1.67 | 0.60 |
| 2:BJ:715:LEU:HG | 2:BJ:716:ASN:H | 1.67 | 0.60 |
| 2:C:145:ALA:HB2 | 2:C:542:THR:HB | 1.83 | 0.60 |
| 5:CG:103:ASN:OD1 | 5:CG:104:VAL:N | 2.33 | 0.60 |
| 5:CG:8:GLY:HA3 | 5:CG:15:THR:HG23 | 1.83 | 0.60 |
| 7:DB:513:ARG:O | 7:DC:441:GLN:N | 2.31 | 0.60 |
| 7:DB:160:MET:SD | 7:DD:165:THR:HG21 | 2.42 | 0.60 |
| 10:DH:222:ILE:O | 10:DH:225:ILE:N | 2.35 | 0.60 |
| 12:DJ:213:ALA:HB3 | 12:GC:104:PHE:HZ | 1.66 | 0.60 |
| 2:C:1030:ILE:HD11 | 3:E:7:ILE:HD11 | 1.84 | 0.60 |
| 1:EA:378:PRO:O | 1:EA:379:LYS:HG2 | 2.02 | 0.60 |
| 2:EC:111:GLN:NE2 | 1:GE:646:LEU:O | 2.35 | 0.60 |
| 2:EC:366:TYR:HB3 | 2:EC:378:LEU:HD11 | 1.84 | 0.60 |
| 2:EC:103:PHE:HZ | 2:EC:626:GLN:O | 1.85 | 0.60 |
| 2:EC:872:SER:O | 2:EC:873:SER:OG | 2.16 | 0.60 |
| 4:EF:171:LYS:HB2 | 4:EG:165:GLU:HB3 | 1.83 | 0.60 |
| 5:EJ:551:ILE:HD13 | 5:FA:565:ILE:HD13 | 1.83 | 0.60 |
| 7:FF:99:ARG:HH12 | 7:FF:101:SER:HB3 | 1.67 | 0.60 |
| 7:FF:212:PRO:HB2 | 7:FG:203:THR:HG22 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:GC:161:SER:HA | 12:GC:240:ASP:HA | 1.83 | 0.60 |
| 2:GF:366:TYR:HB3 | 2:GF:378:LEU:HD11 | 1.84 | 0.60 |
| 4:GI:165:GLU:HB3 | 4:HA:171:LYS:HB2 | 1.83 | 0.60 |
| 4:GJ:193:HIS:HB3 | 4:GJ:196:GLU:HG3 | 1.83 | 0.60 |
| 4:GJ:275:ALA:O | 4:HA:282:GLN:NE2 | 2.35 | 0.60 |
| 5:HB:223:VAL:HB | 5:HB:224:PRO:HD3 | 1.83 | 0.60 |
| 5:HB:30:PHE:HE1 | 5:HD:30:PHE:HE1 | 1.50 | 0.60 |
| 5:HC:318:GLN:HE22 | 6:HE:8:ALA:N | 2.00 | 0.60 |
| 5:HB:517:GLY:N | 5:HD:594:THR:OG1 | 2.35 | 0.60 |
| 5:K:290:SER:HB2 | 5:K:370:HIS:HA | 1.84 | 0.60 |
| 6:L:16:ASP:OD2 | 6:L:45:LYS:NZ | 2.29 | 0.60 |
| 7:O:473:LYS:HE2 | 5:FA:362:GLU:OE2 | 2.00 | 0.60 |
| 12:W:161:SER:HA | 12:W:240:ASP:HA | 1.83 | 0.60 |
| 1:X:116:ASP:OD1 | 1:X:117:ALA:N | 2.35 | 0.60 |
| 1:X:231:ASP:OD1 | 1:X:232:GLY:N | 2.35 | 0.60 |
| 1:Y:209:TRP:O | 1:Y:212:LYS:N | 2.35 | 0.60 |
| 13:YA:320[A]:THR:HB | 13:YA:324[A]:ALA:HB2 | 1.84 | 0.60 |
| 13:YA:437[B]:ASN:HB3 | 13:YA:439[B]:TYR:HE1 | 1.66 | 0.60 |
| 13:YA:397[E]:SER:OG | 13:YB:405[E]:ASP:OD1 | 2.20 | 0.60 |
| 13:YC:534[B]:LEU:HD11 | 13:YC:536[B]:TRP:HE1 | 1.66 | 0.60 |
| 13:YC:65[D]:ALA:N | 13:YC:69[D]:ILE:O | 2.35 | 0.60 |
| 13:YC:58[E]:ILE:HG12 | 13:YC:97[E]:LEU:HD22 | 1.83 | 0.60 |
| 14:YD:118[A]:LEU:HD23 | 14:YD:139[A]:ILE:HD13 | 1.83 | 0.60 |
| 14:YD:41[B]:ARG:HG2 | 14:YD:343[B]:ILE:HG12 | 1.83 | 0.60 |
| 14:YD:35[B]:ILE:HA | 14:YD:54[B]:PHE:HB3 | 1.83 | 0.60 |
| 14:YE:41[B]:ARG:HG2 | 14:YE:343[B]:ILE:HG12 | 1.84 | 0.60 |
| 14:YE:41[E]:ARG:HG2 | 14:YE:343[E]:ILE:HG12 | 1.84 | 0.60 |
| 14:YF:70[C]:ILE:O | 14:YF:88[C]:TYR:N | 2.34 | 0.60 |
| 4:AB:193:HIS:HB3 | 4:AB:196:GLU:HG3 | 1.83 | 0.60 |
| 5:AD:78:THR:HA | 5:AD:108:THR:HB | 1.84 | 0.60 |
| 7:AI:47:VAL:HA | 7:AI:57:ILE:HD12 | 1.83 | 0.60 |
| 7:BA:2:SER:N | 7:BA:5:THR:HG1 | 2.00 | 0.60 |
| 7:BA:333:THR:OG1 | 7:BA:335:ASN:OD1 | 2.18 | 0.60 |
| 8:BB:76:ASP:OD1 | 8:BB:77:GLU:N | 2.35 | 0.60 |
| 1:BH:286:PHE:HB2 | 1:BH:300:ILE:HD11 | 1.84 | 0.60 |
| 2:BJ:589:LYS:HB3 | 2:BJ:592:GLY:O | 2.01 | 0.60 |
| 2:C:1006:ASP:OD1 | 2:C:1007:LEU:N | 2.35 | 0.60 |
| 2:C:316:ASP:HB3 | 2:C:330:LYS:HE2 | 1.84 | 0.60 |
| 3:CA:170:PRO:HG3 | 3:CA:188:TRP:CG | 2.37 | 0.60 |
| 3:CA:75:MET:HG2 | 3:CA:299:PRO:HG3 | 1.84 | 0.60 |
| 2:BJ:1030:ILE:HD11 | 3:CB:7:ILE:HD11 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:102:TRP:HE3 | 5:CH:131:SER:HB2 | 1.67 | 0.60 |
| 5:CH:86:VAL:HG22 | 5:CH:87:ASN:H | 1.67 | 0.60 |
| 7:DD:296:ILE:HG22 | 7:DD:298:GLY:H | 1.67 | 0.60 |
| 8:DF:76:ASP:OD1 | 8:DF:77:GLU:N | 2.35 | 0.60 |
| 2:EC:378:LEU:HD23 | 2:EC:434:MET:HB2 | 1.84 | 0.60 |
| 5:EJ:200:LEU:HD22 | 7:FF:2:SER:HA | 1.84 | 0.60 |
| 5:FA:102:TRP:HE3 | 5:FA:131:SER:HB2 | 1.67 | 0.60 |
| 5:FA:339:GLU:HB3 | 6:FB:172:SER:O | 2.01 | 0.60 |
| 7:FE:29:ILE:HG22 | 7:FE:30:THR:N | 2.14 | 0.60 |
| 7:FF:334:GLN:HG3 | 7:FF:337:ILE:HD12 | 1.84 | 0.60 |
| 7:FG:100:TYR:CD1 | 7:FG:115:SER:HB2 | 2.37 | 0.60 |
| 7:FG:71:ASN:O | 7:FG:73:THR:HG22 | 2.02 | 0.60 |
| 10:DH:143:PHE:CD2 | 10:GA:349:ARG:HD3 | 2.36 | 0.60 |
| 2:GF:378:LEU:HD23 | 2:GF:434:MET:HB2 | 1.84 | 0.60 |
| 2:GF:364:VAL:HG11 | 2:GF:390:PRO:HB3 | 1.82 | 0.60 |
| 4:GI:171:LYS:HB2 | 4:GJ:165:GLU:HB3 | 1.83 | 0.60 |
| 4:GJ:53:GLY:HA2 | 4:GJ:59:GLN:H | 1.66 | 0.60 |
| 5:HC:95:ALA:HB3 | 5:HC:133:LEU:HB2 | 1.82 | 0.60 |
| 5:HC:334:ALA:O | 5:HC:337:ASP:N | 2.35 | 0.60 |
| 7:HJ:2:SER:N | 7:HJ:5:THR:HG1 | 2.00 | 0.60 |
| 7:HJ:4:ASN:OD1 | 7:HJ:15:TYR:OH | 2.17 | 0.60 |
| 5:I:43:PRO:HG2 | 5:K:36:GLU:HG3 | 1.84 | 0.60 |
| 5:J:103:ASN:OD1 | 5:J:104:VAL:N | 2.33 | 0.60 |
| 5:J:213:GLY:HA2 | 5:J:221:GLU:HB2 | 1.83 | 0.60 |
| 5:J:334:ALA:O | 5:J:337:ASP:N | 2.35 | 0.60 |
| 7:O:47:VAL:HA | 7:O:57:ILE:HD12 | 1.83 | 0.60 |
| 7:Q:2:SER:N | 7:Q:5:THR:HG1 | 2.00 | 0.60 |
| 1:Y:539:ARG:H | 1:Y:556:GLY:HA3 | 1.67 | 0.60 |
| 13:YA:534[A]:LEU:HD11 | 13:YA:536[A]:TRP:HE1 | 1.66 | 0.60 |
| 13:YA:534[F]:LEU:HD11 | 13:YA:536[F]:TRP:HE1 | 1.66 | 0.60 |
| 13:YA:58[E]:ILE:HG12 | 13:YA:97[E]:LEU:HD22 | 1.83 | 0.60 |
| 13:YC:76[A]:PRO:HG3 | 13:YC:96[A]:VAL:HB | 1.83 | 0.60 |
| 14:YD:46[E]:GLY:HA3 | 14:YD:174[E]:ARG:HH22 | 1.67 | 0.60 |
| 14:YD:84[B]:LYS:NZ | 14:YD:317[B]:ASN:OD1 | 2.35 | 0.60 |
| 14:YD:70[F]:ILE:O | 14:YD:88[F]:TYR:N | 2.34 | 0.60 |
| 13:YB:47[A]:ILE:HG12 | 14:YE:123[A]:PRO:HD3 | 1.84 | 0.60 |
| 14:YE:125[C]:PHE:CE2 | 14:YE:134[C]:GLU:HG3 | 2.30 | 0.60 |
| 14:YE:46[B]:GLY:HA3 | 14:YE:174[B]:ARG:HH22 | 1.67 | 0.60 |
| 14:YE:41[F]:ARG:HG2 | 14:YE:343[F]:ILE:HG12 | 1.84 | 0.60 |
| 14:YE:184[D]:LYS:HE3 | 14:YE:367[D]:ILE:HG21 | 1.84 | 0.60 |
| 14:YF:46[F]:GLY:HA3 | 14:YF:174[F]:ARG:HH22 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:84[A]:LYS:NZ | 14:YF:317[A]:ASN:OD1 | 2.35 | 0.60 |
| 10:BE:222:ILE:O | 10:BE:225:ILE:N | 2.35 | 0.59 |
| 1:BH:378:PRO:O | 1:BH:379:LYS:HG2 | 2.01 | 0.59 |
| 2:C:150:SER:OG | 2:C:151:PHE:N | 2.33 | 0.59 |
| 2:C:946:SER:O | 2:C:947:VAL:HG22 | 2.02 | 0.59 |
| 3:CA:43:ARG:HH22 | 3:CA:47:TRP:HB3 | 1.66 | 0.59 |
| 5:CG:262:GLN:HG2 | 5:CG:382:ASN:HD22 | 1.66 | 0.59 |
| 3:D:228:ASN:OD1 | 3:D:229:LEU:N | 2.34 | 0.59 |
| 7:DB:260:ARG:NH1 | 7:DD:251:ASN:O | 2.35 | 0.59 |
| 8:DE:125:LYS:HG2 | 8:FH:79:HIS:HB2 | 1.84 | 0.59 |
| 1:EA:231:ASP:OD1 | 1:EA:232:GLY:N | 2.35 | 0.59 |
| 1:EA:526:PRO:HB3 | 13:YA:254[A]:ARG:HD3 | 1.84 | 0.59 |
| 3:EE:114:CYS:HA | 3:EE:120:ASN:HD21 | 1.66 | 0.59 |
| 4:EF:69:LYS:NZ | 4:EG:103:LEU:O | 2.27 | 0.59 |
| 5:EI:3:GLN:HG2 | 5:EI:25:LYS:HG3 | 1.82 | 0.59 |
| 5:EJ:20:ARG:HH12 | 5:EJ:24:ILE:HD12 | 1.67 | 0.59 |
| 7:FF:147:LEU:HB2 | 7:FF:148:PRO:HD3 | 1.84 | 0.59 |
| 8:FH:43:ALA:CB | 8:IA:138:GLY:HA3 | 2.31 | 0.59 |
| 10:GA:222:ILE:O | 10:GA:225:ILE:N | 2.35 | 0.59 |
| 1:GD:336:GLN:HG3 | 1:GD:337:GLN:H | 1.67 | 0.59 |
| 5:HC:176:ASP:HA | 5:HC:231:ARG:HA | 1.84 | 0.59 |
| 6:HE:10:VAL:HA | 6:HF:13:ARG:HD2 | 1.84 | 0.59 |
| 7:HJ:118:PRO:HA | 7:HJ:121:PHE:HB3 | 1.82 | 0.59 |
| 7:HJ:151:LEU:HD12 | 7:HJ:168:LEU:HD22 | 1.83 | 0.59 |
| 7:HH:55:LYS:HB3 | 7:HJ:57:ILE:HG22 | 1.83 | 0.59 |
| 5:I:223:VAL:HB | 5:I:224:PRO:HD3 | 1.83 | 0.59 |
| 5:I:43:PRO:HG3 | 5:K:33:LEU:HA | 1.84 | 0.59 |
| 5:J:206:PHE:CG | 5:J:223:VAL:HA | 2.37 | 0.59 |
| 5:J:20:ARG:HH12 | 5:J:24:ILE:HD12 | 1.67 | 0.59 |
| 5:K:362:GLU:OE2 | 7:AI:473:LYS:HE2 | 2.02 | 0.59 |
| 6:N:95:THR:N | 6:N:174:TYR:O | 2.34 | 0.59 |
| 7:O:55:LYS:HB3 | 7:Q:57:ILE:HG22 | 1.83 | 0.59 |
| 7:Q:7:GLN:HB3 | 7:Q:15:TYR:CZ | 2.36 | 0.59 |
| 8:R:76:ASP:OD1 | 8:R:77:GLU:N | 2.35 | 0.59 |
| 10:U:236:GLU:C | 10:U:287:VAL:HB | 2.22 | 0.59 |
| 12:W:101:LEU:HD23 | 12:IF:253:VAL:HG11 | 1.82 | 0.59 |
| 13:YA:567[B]:ILE:O | 13:YC:575[B]:GLY:N | 2.34 | 0.59 |
| 13:YA:65[A]:ALA:N | 13:YA:69[A]:ILE:O | 2.35 | 0.59 |
| 13:YA:65[E]:ALA:N | 13:YA:69[E]:ILE:O | 2.34 | 0.59 |
| 13:YB:47[F]:ILE:HG12 | 14:YE:123[F]:PRO:HD3 | 1.83 | 0.59 |
| 13:YB:47[C]:ILE:HG23 | 14:YE:123[C]:PRO:CG | 2.30 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:387[B]:TYR:CZ | 13:YC:388[B]:PRO:HB3 | 2.37 | 0.59 |
| 13:YC:437[D]:ASN:HB3 | 13:YC:439[D]:TYR:HE1 | 1.67 | 0.59 |
| 13:YB:468[A]:ASP:HB3 | 13:YC:461[A]:SER:HA | 1.83 | 0.59 |
| 13:YC:50[C]:GLU:N | 13:YC:50[C]:GLU:OE2 | 2.33 | 0.59 |
| 13:YC:534[C]:LEU:HD11 | 13:YC:536[C]:TRP:HE1 | 1.66 | 0.59 |
| 14:YD:118[E]:LEU:HD23 | 14:YD:139[E]:ILE:HD13 | 1.83 | 0.59 |
| 14:YD:294[B]:GLU:O | 14:YD:297[B]:ARG:N | 2.34 | 0.59 |
| 14:YE:118[D]:LEU:HD23 | 14:YE:139[D]:ILE:HD13 | 1.83 | 0.59 |
| 14:YE:41[A]:ARG:HG2 | 14:YE:343[A]:ILE:HG12 | 1.84 | 0.59 |
| 14:YF:41[C]:ARG:HG2 | 14:YF:343[C]:ILE:HG12 | 1.84 | 0.59 |
| 5:AD:151:ILE:HD12 | 5:AD:152:ASP:H | 1.66 | 0.59 |
| 5:AE:290:SER:CB | 5:AE:371:PHE:H | 2.14 | 0.59 |
| 7:AJ:147:LEU:HB2 | 7:AJ:148:PRO:HD3 | 1.84 | 0.59 |
| 1:B:440:ILE:HG22 | 1:B:471:ALA:HB3 | 1.84 | 0.59 |
| 7:BA:386:ASN:OD1 | 7:BA:389:ASN:N | 2.24 | 0.59 |
| 1:BH:116:ASP:OD1 | 1:BH:117:ALA:N | 2.35 | 0.59 |
| 1:BI:209:TRP:O | 1:BI:212:LYS:N | 2.35 | 0.59 |
| 2:BJ:1006:ASP:OD1 | 2:BJ:1007:LEU:N | 2.35 | 0.59 |
| 2:BJ:316:ASP:HB3 | 2:BJ:330:LYS:HE2 | 1.84 | 0.59 |
| 2:C:403:ILE:HG21 | 2:C:417:PHE:HB3 | 1.83 | 0.59 |
| 5:CF:362:GLU:HG3 | 5:CF:363:ASN:N | 2.17 | 0.59 |
| 5:CG:146:VAL:HB | 5:CH:153:LYS:HA | 1.83 | 0.59 |
| 5:CG:65:GLY:O | 5:CH:45:SER:OG | 2.13 | 0.59 |
| 5:CH:331:CYS:HA | 5:CH:349:TRP:HZ2 | 1.67 | 0.59 |
| 5:CG:551:ILE:HD13 | 5:CH:565:ILE:HD13 | 1.82 | 0.59 |
| 7:DD:525:VAL:HG23 | 7:DD:526:LYS:HG2 | 1.84 | 0.59 |
| 1:EA:116:ASP:OD1 | 1:EA:117:ALA:N | 2.35 | 0.59 |
| 1:EB:281:ASN:HA | 1:EB:313:ALA:HB3 | 1.84 | 0.59 |
| 2:EC:145:ALA:HB2 | 2:EC:542:THR:HB | 1.83 | 0.59 |
| 2:EC:403:ILE:HG21 | 2:EC:417:PHE:HB3 | 1.84 | 0.59 |
| 4:EF:43:GLY:O | 4:EF:68:GLN:NE2 | 2.32 | 0.59 |
| 5:EI:154:ILE:HB | 5:FA:156:SER:HB2 | 1.84 | 0.59 |
| 5:EI:362:GLU:HG3 | 5:EI:363:ASN:N | 2.17 | 0.59 |
| 5:EJ:362:GLU:HB2 | 5:EJ:367:GLU:OE1 | 2.03 | 0.59 |
| 5:FA:186:TYR:OH | 5:FA:190:ASN:O | 2.12 | 0.59 |
| 7:FE:117:THR:HG23 | 7:FE:120:LYS:H | 1.66 | 0.59 |
| 7:FE:263:VAL:HG12 | 7:FE:278:SER:HB3 | 1.84 | 0.59 |
| 7:FG:525:VAL:HG23 | 7:FG:526:LYS:HG2 | 1.84 | 0.59 |
| 9:FJ:56:ASP:OD1 | 9:FJ:57:LEU:N | 2.34 | 0.59 |
| 1:GD:206:TRP:CD1 | 1:GD:222:THR:HB | 2.37 | 0.59 |
| 1:GD:441:ILE:HD11 | 1:GD:644:ASN:ND2 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:1006:ASP:OD1 | 2:GF:1007:LEU:N | 2.35 | 0.59 |
| 2:GF:103:PHE:HZ | 2:GF:626:GLN:O | 1.85 | 0.59 |
| 2:GF:185:LYS:HE3 | 2:GF:189:ARG:CZ | 2.31 | 0.59 |
| 2:GF:715:LEU:HG | 2:GF:716:ASN:H | 1.67 | 0.59 |
| 2:GF:921:TRP:NE1 | 5:HC:19:LEU:HA | 2.17 | 0.59 |
| 5:HC:213:GLY:HA2 | 5:HC:221:GLU:HB2 | 1.83 | 0.59 |
| 7:HH:220:SER:OG | 7:HH:226:GLY:O | 2.20 | 0.59 |
| 7:HH:263:VAL:HG12 | 7:HH:278:SER:HB3 | 1.84 | 0.59 |
| 7:HI:211:SER:N | 7:HI:214:THR:OG1 | 2.28 | 0.59 |
| 5:I:285:LEU:HD21 | 5:I:375:PHE:H | 1.68 | 0.59 |
| 8:IB:76:ASP:OD1 | 8:IB:77:GLU:N | 2.35 | 0.59 |
| 11:IE:110:VAL:HG22 | 11:IE:111:TYR:HD2 | 1.68 | 0.59 |
| 5:J:262:GLN:HG2 | 5:J:382:ASN:HD22 | 1.66 | 0.59 |
| 5:K:86:VAL:HG22 | 5:K:87:ASN:H | 1.67 | 0.59 |
| 7:O:96:GLY:N | 7:Q:97:LEU:HB3 | 2.17 | 0.59 |
| 7:Q:296:ILE:HG22 | 7:Q:298:GLY:H | 1.67 | 0.59 |
| 8:S:68:ASP:OD1 | 8:S:69:TRP:N | 2.35 | 0.59 |
| 1:X:278:ALA:HB2 | 1:X:317:GLY:H | 1.67 | 0.59 |
| 1:X:378:PRO:O | 1:X:379:LYS:HG2 | 2.02 | 0.59 |
| 1:X:41:ASN:OD1 | 1:X:42:GLU:N | 2.34 | 0.59 |
| 13:YA:387[F]:TYR:CZ | 13:YA:388[F]:PRO:HB3 | 2.38 | 0.59 |
| 13:YA:397[F]:SER:OG | 13:YB:405[F]:ASP:OD1 | 2.20 | 0.59 |
| 13:YA:76[A]:PRO:HG3 | 13:YA:96[A]:VAL:HB | 1.83 | 0.59 |
| 13:YB:179[F]:MET:SD | 13:YB:279[F]:ASN:ND2 | 2.75 | 0.59 |
| 13:YB:320[E]:THR:HB | 13:YB:324[E]:ALA:HB2 | 1.84 | 0.59 |
| 13:YC:437[A]:ASN:HB3 | 13:YC:439[A]:TYR:HE1 | 1.67 | 0.59 |
| 13:YA:438[A]:LEU:HD22 | 13:YC:442[A]:THR:HG21 | 1.83 | 0.59 |
| 13:YC:57[C]:VAL:CG1 | 13:YC:76[C]:PRO:HD3 | 2.31 | 0.59 |
| 13:YC:76[D]:PRO:HG3 | 13:YC:96[D]:VAL:HB | 1.83 | 0.59 |
| 14:YD:125[E]:PHE:CE2 | 14:YD:134[E]:GLU:HG3 | 2.30 | 0.59 |
| 14:YD:41[A]:ARG:HG2 | 14:YD:343[A]:ILE:HG12 | 1.84 | 0.59 |
| 14:YE:294[F]:GLU:O | 14:YE:297[F]:ARG:N | 2.34 | 0.59 |
| 14:YE:84[F]:LYS:NZ | 14:YE:317[F]:ASN:OD1 | 2.36 | 0.59 |
| 2:Z:981:GLN:HG2 | 2:Z:982:LEU:N | 2.16 | 0.59 |
| 1:A:116:ASP:OD1 | 1:A:117:ALA:N | 2.35 | 0.59 |
| 1:A:231:ASP:OD1 | 1:A:232:GLY:N | 2.35 | 0.59 |
| 1:A:332:LYS:HE3 | 1:A:348:PHE:HE1 | 1.66 | 0.59 |
| 1:A:336:GLN:HG3 | 1:A:337:GLN:H | 1.67 | 0.59 |
| 1:A:552:LYS:HA | 1:A:594:GLU:HA | 1.83 | 0.59 |
| 5:AE:86:VAL:HG22 | 5:AE:87:ASN:H | 1.67 | 0.59 |
| 9:BD:100:ASP:OD1 | 9:BD:101:ASP:N | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:229:THR:OG1 | 1:BH:231:ASP:OD1 | 2.19 | 0.59 |
| 2:BJ:366:TYR:HB3 | 2:BJ:378:LEU:HD11 | 1.84 | 0.59 |
| 2:C:366:TYR:HB3 | 2:C:378:LEU:HD11 | 1.84 | 0.59 |
| 4:CC:131:LYS:N | 4:CC:160:TRP:O | 2.29 | 0.59 |
| 5:CG:206:PHE:CG | 5:CG:223:VAL:HA | 2.37 | 0.59 |
| 5:CG:60:LEU:HG | 5:CG:79:ILE:HG22 | 1.82 | 0.59 |
| 5:CH:290:SER:CB | 5:CH:370:HIS:HA | 2.33 | 0.59 |
| 3:D:253:LEU:HD12 | 3:D:326:GLU:HB2 | 1.83 | 0.59 |
| 7:DB:220:SER:OG | 7:DB:226:GLY:O | 2.20 | 0.59 |
| 7:DD:333:THR:OG1 | 7:DD:335:ASN:OD1 | 2.18 | 0.59 |
| 8:DF:68:ASP:OD1 | 8:DF:69:TRP:N | 2.36 | 0.59 |
| 1:EA:332:LYS:HE3 | 1:EA:348:PHE:HE1 | 1.66 | 0.59 |
| 1:EA:441:ILE:HD11 | 1:EA:644:ASN:ND2 | 2.17 | 0.59 |
| 5:EJ:334:ALA:O | 5:EJ:337:ASP:N | 2.35 | 0.59 |
| 5:EI:517:GLY:N | 5:FA:594:THR:OG1 | 2.36 | 0.59 |
| 6:FB:12:SER:HB3 | 6:FD:6:ASN:HB3 | 1.83 | 0.59 |
| 7:FE:184:THR:OG1 | 7:FE:187:ASP:N | 2.34 | 0.59 |
| 7:FG:12:GLU:HB3 | 7:FG:15:TYR:HB3 | 1.84 | 0.59 |
| 7:FG:151:LEU:HD12 | 7:FG:168:LEU:HD22 | 1.83 | 0.59 |
| 7:FG:7:GLN:HB3 | 7:FG:15:TYR:CZ | 2.36 | 0.59 |
| 8:FI:68:ASP:OD1 | 8:FI:69:TRP:N | 2.36 | 0.59 |
| 1:GE:440:ILE:HD11 | 1:GE:653:ILE:HG12 | 1.85 | 0.59 |
| 3:GG:75:MET:HG2 | 3:GG:299:PRO:HG3 | 1.84 | 0.59 |
| 5:HB:361:ASP:H | 5:HB:366:PRO:HA | 1.66 | 0.59 |
| 5:HC:20:ARG:HH12 | 5:HC:24:ILE:HD12 | 1.67 | 0.59 |
| 7:HI:513:ARG:O | 7:HJ:441:GLN:N | 2.23 | 0.59 |
| 7:HI:97:LEU:HB3 | 7:HJ:95:TYR:HB3 | 1.85 | 0.59 |
| 7:HH:134:SER:HB2 | 7:HJ:143:LYS:HA | 1.84 | 0.59 |
| 5:I:279:SER:HB2 | 5:K:326:MET:HE3 | 1.82 | 0.59 |
| 5:I:367:GLU:N | 5:I:367:GLU:OE1 | 2.36 | 0.59 |
| 5:I:557:TYR:HB2 | 5:I:559:PRO:HD2 | 1.85 | 0.59 |
| 10:ID:222:ILE:O | 10:ID:225:ILE:N | 2.35 | 0.59 |
| 5:K:331:CYS:HA | 5:K:349:TRP:HZ2 | 1.67 | 0.59 |
| 8:R:23:VAL:HB | 8:R:113:VAL:HG23 | 1.84 | 0.59 |
| 1:X:17:ILE:HG22 | 1:X:19:GLU:H | 1.67 | 0.59 |
| 1:X:126:PRO:HD2 | 1:X:292:LEU:HD21 | 1.82 | 0.59 |
| 13:YA:438[D]:LEU:HD22 | 13:YC:442[D]:THR:HG21 | 1.83 | 0.59 |
| 13:YB:179[C]:MET:SD | 13:YB:279[C]:ASN:ND2 | 2.76 | 0.59 |
| 13:YB:468[C]:ASP:HB3 | 13:YC:461[C]:SER:HA | 1.83 | 0.59 |
| 13:YB:47[D]:ILE:HG12 | 14:YE:123[D]:PRO:HD3 | 1.83 | 0.59 |
| 13:YB:534[E]:LEU:HD11 | 13:YB:536[E]:TRP:HE1 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:554[E]:MET:HE2 | 13:YB:550[E]:TRP:CD1 | 2.37 | 0.59 |
| 13:YC:320[C]:THR:HB | 13:YC:324[C]:ALA:HB2 | 1.85 | 0.59 |
| 13:YB:434[C]:THR:HG21 | 13:YC:430[C]:ARG:HB3 | 1.84 | 0.59 |
| 14:YD:125[A]:PHE:CE2 | 14:YD:134[A]:GLU:HG3 | 2.30 | 0.59 |
| 14:YD:232[F]:TYR:OH | 14:YD:312[F]:THR:O | 2.20 | 0.59 |
| 11:BF:190:LYS:HE3 | 14:YD:24[D]:SER:O | 2.02 | 0.59 |
| 14:YD:84[A]:LYS:NZ | 14:YD:317[A]:ASN:OD1 | 2.35 | 0.59 |
| 14:YE:70[D]:ILE:HG21 | 14:YE:109[D]:LEU:HD21 | 1.85 | 0.59 |
| 14:YE:46[C]:GLY:HA3 | 14:YE:174[C]:ARG:HH22 | 1.67 | 0.59 |
| 14:YE:332[B]:GLN:HB3 | 14:YF:61[B]:HIS:CE1 | 2.36 | 0.59 |
| 14:YE:70[D]:ILE:O | 14:YE:88[D]:TYR:N | 2.34 | 0.59 |
| 14:YF:46[A]:GLY:HA3 | 14:YF:174[A]:ARG:HH22 | 1.67 | 0.59 |
| 14:YF:46[E]:GLY:HA3 | 14:YF:174[E]:ARG:HH22 | 1.67 | 0.59 |
| 14:YF:232[A]:TYR:OH | 14:YF:312[A]:THR:O | 2.21 | 0.59 |
| 14:YF:232[F]:TYR:OH | 14:YF:312[F]:THR:O | 2.20 | 0.59 |
| 14:YD:61[C]:HIS:CE1 | 14:YF:332[C]:GLN:HB3 | 2.36 | 0.59 |
| 14:YF:70[B]:ILE:O | 14:YF:88[B]:TYR:N | 2.34 | 0.59 |
| 14:YF:70[E]:ILE:O | 14:YF:88[E]:TYR:N | 2.34 | 0.59 |
| 2:Z:185:LYS:HE3 | 2:Z:189:ARG:CZ | 2.32 | 0.59 |
| 5:AC:223:VAL:HB | 5:AC:224:PRO:HD3 | 1.83 | 0.59 |
| 5:AC:43:PRO:HG2 | 5:AE:36:GLU:HG3 | 1.85 | 0.59 |
| 6:AH:16:ASP:OD2 | 6:AH:45:LYS:NZ | 2.29 | 0.59 |
| 7:AI:263:VAL:HG12 | 7:AI:278:SER:HB3 | 1.84 | 0.59 |
| 7:AI:512:THR:HA | 7:AJ:442:MET:HA | 1.84 | 0.59 |
| 7:AI:55:LYS:HB3 | 7:BA:57:ILE:HG22 | 1.83 | 0.59 |
| 7:BA:100:TYR:CD1 | 7:BA:115:SER:HB2 | 2.37 | 0.59 |
| 7:AJ:36:ILE:HG21 | 7:BA:18:PHE:CZ | 2.35 | 0.59 |
| 7:BA:418:ASP:OD1 | 7:BA:422:LYS:N | 2.28 | 0.59 |
| 8:BC:38:ALA:HB3 | 8:BC:72:THR:HG22 | 1.85 | 0.59 |
| 1:BI:455:PHE:CD1 | 1:BI:639:LEU:HD12 | 2.35 | 0.59 |
| 2:C:149:GLU:O | 2:C:150:SER:OG | 2.18 | 0.59 |
| 5:CG:356:TYR:HE1 | 6:CI:4:LEU:HD13 | 1.67 | 0.59 |
| 5:CG:362:GLU:HB2 | 5:CG:367:GLU:OE1 | 2.03 | 0.59 |
| 5:CF:569:TYR:H | 5:CG:550:VAL:HB | 1.67 | 0.59 |
| 5:CH:196:ARG:NH1 | 7:DC:8:HIS:HB3 | 2.17 | 0.59 |
| 6:CI:75:THR:HB | 7:FF:167:GLN:HE22 | 1.67 | 0.59 |
| 3:D:170:PRO:HG3 | 3:D:188:TRP:CG | 2.37 | 0.59 |
| 7:DB:186:SER:O | 7:DD:192:GLN:NE2 | 2.35 | 0.59 |
| 10:DH:129:LEU:HD11 | 10:DH:225:ILE:HD11 | 1.83 | 0.59 |
| 5:FA:316:ILE:HG21 | 6:FC:7:LYS:HG3 | 1.84 | 0.59 |
| 7:FE:309:ALA:HB3 | 7:FG:303:GLU:HA | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FH:76:ASP:OD1 | 8:FH:77:GLU:N | 2.35 | 0.59 |
| 8:FI:89:GLN:HB3 | 8:FI:134:PRO:HG2 | 1.85 | 0.59 |
| 1:GE:102:SER:N | 1:GE:194:ARG:HH12 | 2.00 | 0.59 |
| 1:GE:209:TRP:O | 1:GE:212:LYS:N | 2.35 | 0.59 |
| 4:GI:193:HIS:HB3 | 4:GI:196:GLU:HG3 | 1.83 | 0.59 |
| 5:HC:146:VAL:HB | 5:HD:153:LYS:HA | 1.84 | 0.59 |
| 5:HC:260:ARG:O | 5:HC:261:ARG:NH1 | 2.33 | 0.59 |
| 6:HG:95:THR:N | 6:HG:174:TYR:O | 2.34 | 0.59 |
| 7:HH:212:PRO:HG3 | 7:HI:199:VAL:HG12 | 1.85 | 0.59 |
| 6:FB:77:VAL:HG23 | 7:HI:167:GLN:NE2 | 2.17 | 0.59 |
| 7:HJ:7:GLN:HB3 | 7:HJ:15:TYR:CZ | 2.36 | 0.59 |
| 5:I:557:TYR:OH | 5:J:556:GLN:OE1 | 2.21 | 0.59 |
| 5:I:569:TYR:H | 5:J:550:VAL:HB | 1.67 | 0.59 |
| 8:IB:68:ASP:OD1 | 8:IB:69:TRP:N | 2.36 | 0.59 |
| 11:IE:190:LYS:HE3 | 14:YD:24[A]:SER:O | 2.02 | 0.59 |
| 6:L:58:ASP:OD1 | 6:M:164:GLN:NE2 | 2.36 | 0.59 |
| 1:X:206:TRP:CD1 | 1:X:222:THR:HB | 2.37 | 0.59 |
| 13:YA:437[F]:ASN:HB3 | 13:YA:439[F]:TYR:HE1 | 1.66 | 0.59 |
| 13:YA:572[C]:ILE:O | 15:ZA:68[C]:TYR:HB2 | 2.03 | 0.59 |
| 13:YA:65[D]:ALA:N | 13:YA:69[D]:ILE:O | 2.35 | 0.59 |
| 13:YB:387[B]:TYR:CZ | 13:YB:388[B]:PRO:HB3 | 2.37 | 0.59 |
| 13:YB:534[D]:LEU:HD11 | 13:YB:536[D]:TRP:HE1 | 1.66 | 0.59 |
| 13:YB:58[E]:ILE:HG12 | 13:YB:97[E]:LEU:HD22 | 1.83 | 0.59 |
| 13:YC:193[B]:ASP:OD1 | 13:YC:197[B]:TYR:N | 2.33 | 0.59 |
| 13:YC:320[A]:THR:HB | 13:YC:324[A]:ALA:HB2 | 1.84 | 0.59 |
| 13:YC:61[F]:ILE:HG13 | 13:YC:62[F]:THR:N | 2.17 | 0.59 |
| 14:YD:232[E]:TYR:OH | 14:YD:312[E]:THR:O | 2.21 | 0.59 |
| 14:YE:84[C]:LYS:NZ | 14:YE:317[C]:ASN:OD1 | 2.36 | 0.59 |
| 14:YE:70[A]:ILE:O | 14:YE:88[A]:TYR:N | 2.34 | 0.59 |
| 14:YF:125[C]:PHE:CE2 | 14:YF:134[C]:GLU:HG3 | 2.30 | 0.59 |
| 1:Y:214:MET:N | 2:Z:733:ASP:OD2 | 2.34 | 0.59 |
| 5:AC:362:GLU:HG3 | 5:AC:363:ASN:N | 2.17 | 0.59 |
| 5:AC:472:TYR:HB3 | 5:AD:418:GLY:C | 2.23 | 0.59 |
| 5:AE:290:SER:CB | 5:AE:370:HIS:HA | 2.33 | 0.59 |
| 7:AJ:99:ARG:HH12 | 7:AJ:101:SER:HB3 | 1.67 | 0.59 |
| 7:AJ:334:GLN:HG3 | 7:AJ:337:ILE:HD12 | 1.85 | 0.59 |
| 8:BC:76:ASP:OD1 | 8:BC:77:GLU:N | 2.35 | 0.59 |
| 10:BE:288:SER:OG | 10:BE:289:ASN:N | 2.36 | 0.59 |
| 1:BH:278:ALA:HB2 | 1:BH:317:GLY:H | 1.67 | 0.59 |
| 2:BJ:1012:LEU:HD13 | 2:BJ:1027:GLN:NE2 | 2.18 | 0.59 |
| 2:C:185:LYS:HE3 | 2:C:189:ARG:CZ | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:49:LEU:HB3 | 2:C:50:PRO:HD3 | 1.85 | 0.59 |
| 5:CF:322:GLY:N | 5:CF:358:VAL:O | 2.36 | 0.59 |
| 5:CF:367:GLU:OE1 | 5:CF:367:GLU:N | 2.36 | 0.59 |
| 5:CF:71:ASN:OD1 | 5:CF:73:SER:N | 2.27 | 0.59 |
| 5:CG:316:ILE:HG23 | 5:CH:315:GLY:HA3 | 1.85 | 0.59 |
| 5:CH:359:GLU:HB3 | 5:CH:370:HIS:HB3 | 1.84 | 0.59 |
| 5:CF:520:GLY:O | 5:CH:591:PRO:HA | 2.03 | 0.59 |
| 7:DB:326:ILE:HG23 | 7:DD:323:GLY:HA2 | 1.83 | 0.59 |
| 8:DE:76:ASP:OD1 | 8:DE:77:GLU:N | 2.35 | 0.59 |
| 10:DH:288:SER:OG | 10:DH:289:ASN:N | 2.36 | 0.59 |
| 5:EI:285:LEU:HD21 | 5:EI:375:PHE:H | 1.68 | 0.59 |
| 5:EI:290:SER:CB | 5:EI:370:HIS:HA | 2.31 | 0.59 |
| 5:FA:331:CYS:HA | 5:FA:349:TRP:HZ2 | 1.67 | 0.59 |
| 5:FA:290:SER:CB | 5:FA:370:HIS:HA | 2.33 | 0.59 |
| 6:FC:17:PHE:O | 6:FD:13:ARG:NH1 | 2.26 | 0.59 |
| 7:FG:20:PRO:HB3 | 7:FG:29:ILE:HG13 | 1.84 | 0.59 |
| 7:FE:297:TYR:N | 7:FG:290:GLN:O | 2.27 | 0.59 |
| 10:GA:129:LEU:HD11 | 10:GA:225:ILE:HD11 | 1.83 | 0.59 |
| 1:GE:200:TYR:HB2 | 1:GE:269:VAL:CG1 | 2.33 | 0.59 |
| 2:GF:64:ASN:OD1 | 2:GF:65:ASN:N | 2.34 | 0.59 |
| 5:HD:290:SER:HB2 | 5:HD:370:HIS:HA | 1.84 | 0.59 |
| 7:HH:218:SER:O | 7:HH:227:VAL:HG22 | 2.02 | 0.59 |
| 7:HH:192:GLN:NE2 | 7:HI:186:SER:O | 2.35 | 0.59 |
| 7:HH:481:SER:OG | 7:HI:449:GLY:O | 2.13 | 0.59 |
| 7:HI:73:THR:HG23 | 7:HI:74:LYS:H | 1.68 | 0.59 |
| 7:HJ:100:TYR:CD1 | 7:HJ:115:SER:HB2 | 2.37 | 0.59 |
| 7:HJ:71:ASN:O | 7:HJ:73:THR:HG22 | 2.01 | 0.59 |
| 5:I:34:TYR:O | 5:I:38:GLY:N | 2.26 | 0.59 |
| 10:ID:236:GLU:C | 10:ID:287:VAL:HB | 2.22 | 0.59 |
| 7:O:160:MET:SD | 7:Q:165:THR:HG21 | 2.42 | 0.59 |
| 7:O:263:VAL:HG12 | 7:O:278:SER:HB3 | 1.84 | 0.59 |
| 8:S:38:ALA:HB3 | 8:S:72:THR:HG22 | 1.85 | 0.59 |
| 9:T:100:ASP:OD1 | 9:T:101:ASP:N | 2.34 | 0.59 |
| 13:YA:558[F]:SER:HB3 | 13:YB:551[F]:THR:HG22 | 1.84 | 0.59 |
| 13:YA:397[A]:SER:OG | 13:YB:405[A]:ASP:OD1 | 2.21 | 0.59 |
| 13:YA:397[B]:SER:OG | 13:YB:405[B]:ASP:OD1 | 2.20 | 0.59 |
| 13:YB:434[D]:THR:HG21 | 13:YC:430[D]:ARG:HB3 | 1.84 | 0.59 |
| 13:YA:438[C]:LEU:HD22 | 13:YC:442[C]:THR:HG21 | 1.83 | 0.59 |
| 13:YC:534[E]:LEU:HD11 | 13:YC:536[E]:TRP:HE1 | 1.66 | 0.59 |
| 13:YC:57[B]:VAL:CG1 | 13:YC:76[B]:PRO:HD3 | 2.32 | 0.59 |
| 14:YD:46[D]:GLY:HA3 | 14:YD:174[D]:ARG:HH22 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:70[D]:ILE:HG21 | 14:YD:109[D]:LEU:HD21 | 1.85 | 0.59 |
| 14:YD:84[E]:LYS:NZ | 14:YD:317[E]:ASN:OD1 | 2.36 | 0.59 |
| 14:YE:245[C]:ARG:NE | 14:YE:246[C]:ASP:OD1 | 2.25 | 0.59 |
| 2:Z:64:ASN:OD1 | 2:Z:65:ASN:N | 2.34 | 0.59 |
| 2:Z:703:TYR:O | 2:Z:706:SER:N | 2.31 | 0.59 |
| 5:AD:206:PHE:CG | 5:AD:223:VAL:HA | 2.37 | 0.59 |
| 5:AE:290:SER:HB2 | 5:AE:370:HIS:HA | 1.84 | 0.59 |
| 5:AE:371:PHE:CZ | 5:AE:373:SER:HB3 | 2.38 | 0.59 |
| 6:AF:95:THR:N | 6:AF:174:TYR:O | 2.34 | 0.59 |
| 6:AG:95:THR:N | 6:AG:174:TYR:O | 2.34 | 0.59 |
| 7:BA:525:VAL:HG23 | 7:BA:526:LYS:HG2 | 1.84 | 0.59 |
| 7:BA:47:VAL:HA | 7:BA:57:ILE:HD12 | 1.85 | 0.59 |
| 7:AI:96:GLY:N | 7:BA:97:LEU:HB3 | 2.18 | 0.59 |
| 12:BG:213:ALA:HB3 | 12:DJ:104:PHE:HZ | 1.67 | 0.59 |
| 1:BH:206:TRP:CD1 | 1:BH:222:THR:HB | 2.37 | 0.59 |
| 2:BJ:316:ASP:O | 2:BJ:331:THR:N | 2.34 | 0.59 |
| 3:CA:253:LEU:HD12 | 3:CA:326:GLU:HB2 | 1.83 | 0.59 |
| 4:CD:53:GLY:HA2 | 4:CD:59:GLN:H | 1.66 | 0.59 |
| 5:CG:150:GLN:HB2 | 5:CG:152:ASP:HB3 | 1.84 | 0.59 |
| 7:DB:162:PRO:HB2 | 7:DC:150:ALA:HA | 1.83 | 0.59 |
| 7:DB:263:VAL:HG12 | 7:DB:278:SER:HB3 | 1.84 | 0.59 |
| 7:DB:20:PRO:CD | 7:DB:29:ILE:HG21 | 2.33 | 0.59 |
| 7:DC:99:ARG:HD2 | 7:DD:95:TYR:HE1 | 1.67 | 0.59 |
| 8:DF:23:VAL:HB | 8:DF:113:VAL:HG23 | 1.84 | 0.59 |
| 1:EA:206:TRP:CD1 | 1:EA:222:THR:HB | 2.37 | 0.59 |
| 1:EA:423:THR:O | 1:EA:476:ILE:N | 2.35 | 0.59 |
| 2:EC:1006:ASP:OD1 | 2:EC:1007:LEU:N | 2.35 | 0.59 |
| 2:EC:529:SER:H | 3:GH:233:GLN:HE22 | 1.49 | 0.59 |
| 2:EC:816:LEU:H | 3:EE:201:ASN:ND2 | 2.01 | 0.59 |
| 2:EC:921:TRP:NE1 | 5:EJ:19:LEU:HA | 2.15 | 0.59 |
| 3:ED:75:MET:HG2 | 3:ED:299:PRO:HG3 | 1.84 | 0.59 |
| 5:EI:323:THR:HG23 | 5:EI:359:GLU:HB2 | 1.83 | 0.59 |
| 5:EI:367:GLU:OE1 | 5:EI:367:GLU:N | 2.36 | 0.59 |
| 5:EJ:60:LEU:HG | 5:EJ:79:ILE:HG22 | 1.82 | 0.59 |
| 4:F:42:PHE:O | 4:F:62:HIS:ND1 | 2.27 | 0.59 |
| 7:FE:514:PRO:HB3 | 7:FF:512:THR:O | 2.03 | 0.59 |
| 1:GD:126:PRO:HD2 | 1:GD:292:LEU:HD21 | 1.82 | 0.59 |
| 1:GD:332:LYS:HE3 | 1:GD:348:PHE:HE1 | 1.66 | 0.59 |
| 1:GE:214:MET:N | 2:GF:733:ASP:OD2 | 2.34 | 0.59 |
| 1:GE:330:THR:O | 1:GE:333:ARG:HG2 | 2.03 | 0.59 |
| 2:GF:946:SER:O | 2:GF:947:VAL:HG22 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:GJ:43:GLY:O | 4:GJ:68:GLN:NE2 | 2.32 | 0.59 |
| 5:HB:557:TYR:OH | 5:HC:556:GLN:OE1 | 2.20 | 0.59 |
| 6:HF:57:ASN:HB2 | 6:HG:164:GLN:NE2 | 2.18 | 0.59 |
| 6:HG:16:ASP:OD2 | 6:HG:45:LYS:NZ | 2.29 | 0.59 |
| 7:HI:263:VAL:O | 7:HJ:255:SER:OG | 2.14 | 0.59 |
| 7:FF:71:ASN:CB | 7:HJ:365:GLY:HA2 | 2.32 | 0.59 |
| 7:HJ:77:THR:HG23 | 7:HJ:79:ALA:N | 2.17 | 0.59 |
| 7:HH:96:GLY:N | 7:HJ:97:LEU:HB3 | 2.18 | 0.59 |
| 9:IC:85:GLU:OE2 | 9:IC:87:ARG:NE | 2.29 | 0.59 |
| 12:GC:137:TYR:OH | 12:IF:157:PRO:HD3 | 2.03 | 0.59 |
| 12:GC:20:ASN:OD1 | 12:IF:233:ASP:HA | 2.03 | 0.59 |
| 5:J:8:GLY:HA3 | 5:J:15:THR:HG23 | 1.83 | 0.59 |
| 5:J:4:ASN:OD1 | 5:J:5:ILE:N | 2.36 | 0.59 |
| 6:L:95:THR:N | 6:L:174:TYR:O | 2.34 | 0.59 |
| 7:Q:145:SER:O | 7:Q:164:LYS:NZ | 2.25 | 0.59 |
| 7:Q:77:THR:HG23 | 7:Q:79:ALA:N | 2.17 | 0.59 |
| 1:Y:330:THR:O | 1:Y:333:ARG:HG2 | 2.03 | 0.59 |
| 13:YA:65[B]:ALA:N | 13:YA:69[B]:ILE:O | 2.35 | 0.59 |
| 13:YA:65[C]:ALA:N | 13:YA:69[C]:ILE:O | 2.36 | 0.59 |
| 13:YA:76[D]:PRO:HB2 | 13:YA:98[D]:GLY:N | 2.18 | 0.59 |
| 13:YB:179[E]:MET:SD | 13:YB:279[E]:ASN:ND2 | 2.76 | 0.59 |
| 13:YB:76[D]:PRO:HB2 | 13:YB:98[D]:GLY:N | 2.18 | 0.59 |
| 13:YC:50[D]:GLU:N | 13:YC:50[D]:GLU:OE2 | 2.33 | 0.59 |
| 13:YC:65[A]:ALA:N | 13:YC:69[A]:ILE:O | 2.35 | 0.59 |
| 14:YD:118[F]:LEU:HD23 | 14:YD:139[F]:ILE:HD13 | 1.84 | 0.59 |
| 14:YD:245[E]:ARG:NE | 14:YD:246[E]:ASP:OD1 | 2.25 | 0.59 |
| 14:YD:61[D]:HIS:CE1 | 14:YF:332[D]:GLN:HB3 | 2.38 | 0.59 |
| 14:YD:70[C]:ILE:O | 14:YD:88[C]:TYR:N | 2.34 | 0.59 |
| 14:YE:118[E]:LEU:HD23 | 14:YE:139[E]:ILE:HD13 | 1.84 | 0.59 |
| 13:YB:47[B]:ILE:HG12 | 14:YE:123[B]:PRO:HD3 | 1.85 | 0.59 |
| 14:YE:125[E]:PHE:CE2 | 14:YE:134[E]:GLU:HG3 | 2.30 | 0.59 |
| 14:YE:232[D]:TYR:OH | 14:YE:312[D]:THR:O | 2.21 | 0.59 |
| 14:YE:84[A]:LYS:NZ | 14:YE:317[A]:ASN:OD1 | 2.35 | 0.59 |
| 14:YE:84[B]:LYS:NZ | 14:YE:317[B]:ASN:OD1 | 2.35 | 0.59 |
| 14:YF:245[A]:ARG:NE | 14:YF:246[A]:ASP:OD1 | 2.25 | 0.59 |
| 14:YD:61[F]:HIS:CE1 | 14:YF:332[F]:GLN:HB3 | 2.37 | 0.59 |
| 14:YF:84[D]:LYS:NZ | 14:YF:317[D]:ASN:OD1 | 2.36 | 0.59 |
| 2:Z:211:VAL:N | 2:Z:220:LYS:O | 2.27 | 0.59 |
| 2:Z:366:TYR:HB3 | 2:Z:378:LEU:HD11 | 1.84 | 0.59 |
| 2:Z:49:LEU:HB3 | 2:Z:50:PRO:HD3 | 1.85 | 0.59 |
| 13:YA:572[D]:ILE:O | 15:ZA:68[D]:TYR:HB2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:411:PRO:HG2 | 1:A:413:TYR:CD2 | 2.37 | 0.59 |
| 7:AJ:422:LYS:NZ | 7:BA:498:SER:O | 2.36 | 0.59 |
| 7:BA:77:THR:HG23 | 7:BA:79:ALA:N | 2.17 | 0.59 |
| 8:BB:68:ASP:OD1 | 8:BB:69:TRP:N | 2.36 | 0.59 |
| 10:BE:37:GLN:OE1 | 10:BE:37:GLN:N | 2.36 | 0.59 |
| 1:BH:338:ARG:NH2 | 1:BI:340:VAL:O | 2.35 | 0.59 |
| 1:BI:440:ILE:HD11 | 1:BI:653:ILE:HG12 | 1.85 | 0.59 |
| 2:C:376:PHE:HZ | 2:C:441:VAL:HG11 | 1.65 | 0.59 |
| 2:C:578:PHE:CE2 | 2:C:582:ALA:HB2 | 2.38 | 0.59 |
| 5:CF:139:ALA:HB3 | 5:CG:99:PHE:HB3 | 1.85 | 0.59 |
| 5:CF:223:VAL:HB | 5:CF:224:PRO:HD3 | 1.83 | 0.59 |
| 5:CG:188:VAL:HG23 | 5:CG:225:LEU:HD22 | 1.85 | 0.59 |
| 5:CH:213:GLY:O | 5:CH:214:SER:OG | 2.19 | 0.59 |
| 5:CF:459:ILE:HD11 | 5:CH:463:ALA:HB2 | 1.83 | 0.59 |
| 3:D:294:LYS:HB2 | 3:D:297:TYR:CZ | 2.38 | 0.59 |
| 7:DB:43:GLY:O | 7:DC:42:ALA:HB3 | 2.02 | 0.59 |
| 7:DD:100:TYR:CD1 | 7:DD:115:SER:HB2 | 2.37 | 0.59 |
| 7:DB:140:GLY:HA2 | 7:DD:129:PHE:CZ | 2.37 | 0.59 |
| 7:DD:20:PRO:HB3 | 7:DD:29:ILE:HG13 | 1.84 | 0.59 |
| 7:DD:77:THR:HG23 | 7:DD:79:ALA:N | 2.17 | 0.59 |
| 12:DJ:161:SER:HB3 | 12:DJ:240:ASP:HB3 | 1.85 | 0.59 |
| 1:EA:582:ASN:OD1 | 1:EA:585:GLY:N | 2.27 | 0.59 |
| 3:ED:294:LYS:HB2 | 3:ED:297:TYR:CZ | 2.38 | 0.59 |
| 4:EH:131:LYS:N | 4:EH:160:TRP:O | 2.29 | 0.59 |
| 5:EJ:206:PHE:CG | 5:EJ:223:VAL:HA | 2.37 | 0.59 |
| 5:EJ:310:GLU:HB2 | 5:EJ:384:THR:HB | 1.84 | 0.59 |
| 5:EI:30:PHE:HE1 | 5:FA:30:PHE:CE1 | 2.21 | 0.59 |
| 7:FE:101:SER:OG | 7:FE:106:ALA:N | 2.36 | 0.59 |
| 7:FE:47:VAL:HA | 7:FE:57:ILE:HD12 | 1.83 | 0.59 |
| 7:FE:163:LEU:HB2 | 7:FF:153:GLY:O | 2.03 | 0.59 |
| 12:DJ:149:ARG:HB2 | 10:GA:341:THR:HG21 | 1.85 | 0.59 |
| 1:GD:278:ALA:HB2 | 1:GD:317:GLY:H | 1.67 | 0.59 |
| 1:GD:53:LEU:O | 1:GD:53:LEU:HD12 | 2.03 | 0.59 |
| 3:GG:135:ASP:OD1 | 3:GG:136:VAL:N | 2.34 | 0.59 |
| 4:GJ:42:PHE:O | 4:GJ:62:HIS:ND1 | 2.27 | 0.59 |
| 5:HB:264:ARG:HB3 | 5:HD:326:MET:CE | 2.32 | 0.59 |
| 5:HC:362:GLU:HB2 | 5:HC:367:GLU:OE1 | 2.03 | 0.59 |
| 6:HE:73:ASN:HA | 6:HG:70:ILE:HG12 | 1.83 | 0.59 |
| 7:HH:163:LEU:HB2 | 7:HI:153:GLY:O | 2.03 | 0.59 |
| 7:HI:334:GLN:HG3 | 7:HI:337:ILE:HD12 | 1.84 | 0.59 |
| 8:IA:89:GLN:HB3 | 8:IA:134:PRO:HG2 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:151:ILE:HD12 | 5:J:152:ASP:H | 1.66 | 0.59 |
| 7:O:29:ILE:HG22 | 7:O:30:THR:N | 2.14 | 0.59 |
| 7:O:212:PRO:HG3 | 7:P:199:VAL:HG12 | 1.85 | 0.59 |
| 7:P:99:ARG:HD2 | 7:Q:95:TYR:HE1 | 1.66 | 0.59 |
| 8:R:68:ASP:OD1 | 8:R:69:TRP:N | 2.36 | 0.59 |
| 8:R:38:ALA:HB3 | 8:R:72:THR:HG22 | 1.85 | 0.59 |
| 11:V:110:VAL:HG22 | 11:V:111:TYR:HD2 | 1.67 | 0.59 |
| 1:X:441:ILE:HD11 | 1:X:644:ASN:ND2 | 2.17 | 0.59 |
| 1:Y:102:SER:N | 1:Y:194:ARG:HH12 | 2.00 | 0.59 |
| 1:A:526:PRO:HB3 | 13:YA:254[C]:ARG:HD3 | 1.84 | 0.59 |
| 13:YA:320[E]:THR:HB | 13:YA:324[E]:ALA:HB2 | 1.84 | 0.59 |
| 13:YA:397[D]:SER:OG | 13:YB:405[D]:ASP:OD1 | 2.21 | 0.59 |
| 13:YA:50[C]:GLU:N | 13:YA:50[C]:GLU:OE2 | 2.33 | 0.59 |
| 13:YA:534[C]:LEU:HD11 | 13:YA:536[C]:TRP:HE1 | 1.66 | 0.59 |
| 13:YA:572[A]:ILE:O | 15:ZA:68[A]:TYR:HB2 | 2.03 | 0.59 |
| 13:YA:61[A]:ILE:HA | 13:YB:76[A]:PRO:C | 2.22 | 0.59 |
| 13:YA:61[D]:ILE:HA | 13:YB:76[D]:PRO:C | 2.22 | 0.59 |
| 13:YA:61[F]:ILE:HA | 13:YB:76[F]:PRO:C | 2.22 | 0.59 |
| 13:YA:25[C]:GLY:HA3 | 13:YA:73[C]:VAL:HG12 | 1.84 | 0.59 |
| 13:YB:320[C]:THR:HB | 13:YB:324[C]:ALA:HB2 | 1.84 | 0.59 |
| 13:YB:387[D]:TYR:CZ | 13:YB:388[D]:PRO:HB3 | 2.38 | 0.59 |
| 13:YB:416[A]:HIS:CD2 | 13:YB:418[A]:THR:H | 2.21 | 0.59 |
| 13:YB:416[F]:HIS:CD2 | 13:YB:418[F]:THR:H | 2.21 | 0.59 |
| 13:YB:434[E]:THR:HG21 | 13:YC:430[E]:ARG:HB3 | 1.85 | 0.59 |
| 13:YB:534[A]:LEU:HD11 | 13:YB:536[A]:TRP:HE1 | 1.66 | 0.59 |
| 13:YB:61[A]:ILE:HG21 | 13:YC:59[A]:GLN:CA | 2.24 | 0.59 |
| 13:YB:65[D]:ALA:N | 13:YB:69[D]:ILE:O | 2.35 | 0.59 |
| 13:YC:387[F]:TYR:CZ | 13:YC:388[F]:PRO:HB3 | 2.37 | 0.59 |
| 13:YB:468[F]:ASP:HB3 | 13:YC:461[F]:SER:HA | 1.83 | 0.59 |
| 13:YC:50[A]:GLU:N | 13:YC:50[A]:GLU:OE2 | 2.33 | 0.59 |
| 13:YA:534[C]:LEU:HB2 | 13:YC:538[C]:VAL:HG11 | 1.84 | 0.59 |
| 13:YA:555[F]:ALA:O | 13:YC:563[F]:GLY:N | 2.36 | 0.59 |
| 14:YD:46[C]:GLY:HA3 | 14:YD:174[C]:ARG:HH22 | 1.68 | 0.59 |
| 14:YD:232[D]:TYR:OH | 14:YD:312[D]:THR:O | 2.21 | 0.59 |
| 11:DI:190:LYS:HE3 | 14:YD:24[E]:SER:O | 2.02 | 0.59 |
| 14:YD:41[E]:ARG:HG2 | 14:YD:343[E]:ILE:HG12 | 1.83 | 0.59 |
| 14:YE:46[A]:GLY:HA3 | 14:YE:174[A]:ARG:HH22 | 1.68 | 0.59 |
| 14:YE:232[A]:TYR:OH | 14:YE:312[A]:THR:O | 2.21 | 0.59 |
| 14:YE:232[C]:TYR:OH | 14:YE:312[C]:THR:O | 2.21 | 0.59 |
| 14:YE:41[C]:ARG:HG2 | 14:YE:343[C]:ILE:HG12 | 1.84 | 0.59 |
| 14:YF:232[E]:TYR:OH | 14:YF:312[E]:THR:O | 2.21 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:84[F]:LYS:NZ | 14:YF:317[F]:ASN:OD1 | 2.35 | 0.59 |
| 2:Z:578:PHE:CE2 | 2:Z:582:ALA:HB2 | 2.38 | 0.59 |
| 2:Z:715:LEU:HG | 2:Z:716:ASN:H | 1.67 | 0.59 |
| 13:YA:572[B]:ILE:O | 15:ZA:68[B]:TYR:HB2 | 2.03 | 0.59 |
| 1:A:145:PHE:CB | 1:A:169:GLN:HA | 2.32 | 0.59 |
| 1:A:206:TRP:CD1 | 1:A:222:THR:HB | 2.37 | 0.59 |
| 4:AB:40:ASN:HB3 | 4:AB:45:GLN:HG2 | 1.85 | 0.59 |
| 5:AC:117:ILE:HA | 5:AC:143:TRP:HB2 | 1.85 | 0.59 |
| 5:AC:3:GLN:HG2 | 5:AC:25:LYS:HG3 | 1.82 | 0.59 |
| 5:AC:285:LEU:HD21 | 5:AC:375:PHE:H | 1.68 | 0.59 |
| 5:AD:150:GLN:HB2 | 5:AD:152:ASP:HB3 | 1.84 | 0.59 |
| 5:AD:216:GLY:H | 5:AD:231:ARG:HB2 | 1.68 | 0.59 |
| 5:AD:62:ALA:HB1 | 5:AD:82:PRO:HG3 | 1.85 | 0.59 |
| 7:AI:20:PRO:CD | 7:AI:29:ILE:HG21 | 2.33 | 0.59 |
| 7:AI:162:PRO:HB2 | 7:AJ:150:ALA:HA | 1.84 | 0.59 |
| 10:BE:332:LEU:HD21 | 10:BE:340:SER:HB3 | 1.85 | 0.59 |
| 1:BH:231:ASP:OD1 | 1:BH:232:GLY:N | 2.35 | 0.59 |
| 1:BH:552:LYS:HA | 1:BH:594:GLU:HA | 1.83 | 0.59 |
| 2:C:111:GLN:NE2 | 1:Y:646:LEU:O | 2.36 | 0.59 |
| 5:CF:117:ILE:HA | 5:CF:143:TRP:HB2 | 1.85 | 0.59 |
| 5:CH:92:VAL:HG12 | 5:CH:136:VAL:HG12 | 1.85 | 0.59 |
| 5:CF:43:PRO:HG2 | 5:CH:36:GLU:HG3 | 1.85 | 0.59 |
| 3:D:135:ASP:OD1 | 3:D:136:VAL:N | 2.35 | 0.59 |
| 3:D:95:TRP:CH2 | 3:D:169:PRO:HD3 | 2.38 | 0.59 |
| 7:DB:144:ILE:HG21 | 7:DC:156:ASP:O | 2.03 | 0.59 |
| 1:EA:336:GLN:HG3 | 1:EA:337:GLN:H | 1.67 | 0.59 |
| 4:EF:239:ARG:HD2 | 4:EF:249:ILE:HD12 | 1.85 | 0.59 |
| 5:EI:117:ILE:HA | 5:EI:143:TRP:HB2 | 1.85 | 0.59 |
| 5:EI:322:GLY:N | 5:EI:358:VAL:O | 2.36 | 0.59 |
| 5:FA:92:VAL:HG12 | 5:FA:136:VAL:HG12 | 1.85 | 0.59 |
| 11:GB:110:VAL:HG22 | 11:GB:111:TYR:HD2 | 1.68 | 0.59 |
| 2:GF:154:SER:OG | 2:GF:156:SER:OG | 2.13 | 0.59 |
| 2:GF:49:LEU:HB3 | 2:GF:50:PRO:HD3 | 1.85 | 0.59 |
| 2:GF:333:ASN:CB | 4:GI:18:ALA:HA | 2.30 | 0.59 |
| 5:HB:117:ILE:HA | 5:HB:143:TRP:HB2 | 1.85 | 0.59 |
| 5:HB:139:ALA:HB3 | 5:HC:99:PHE:HB3 | 1.85 | 0.59 |
| 5:HB:577:ASN:ND2 | 5:HC:529:ASN:OD1 | 2.23 | 0.59 |
| 5:HC:62:ALA:HB1 | 5:HC:82:PRO:HG3 | 1.85 | 0.59 |
| 5:HD:290:SER:CB | 5:HD:370:HIS:HA | 2.33 | 0.59 |
| 7:HH:449:GLY:N | 7:HJ:482:TYR:O | 2.32 | 0.59 |
| 5:I:183:GLY:HA2 | 5:I:307:ASN:HD22 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:361:ASP:H | 5:I:366:PRO:HA | 1.66 | 0.59 |
| 5:J:131:SER:HA | 5:J:150:GLN:HA | 1.85 | 0.59 |
| 5:J:139:ALA:HB3 | 5:K:99:PHE:HB3 | 1.84 | 0.59 |
| 7:O:163:LEU:HB2 | 7:P:153:GLY:O | 2.02 | 0.59 |
| 7:P:422:LYS:NZ | 7:Q:498:SER:O | 2.35 | 0.59 |
| 1:X:145:PHE:CB | 1:X:169:GLN:HA | 2.32 | 0.59 |
| 1:X:411:PRO:HG2 | 1:X:413:TYR:CD2 | 2.37 | 0.59 |
| 13:YA:434[A]:THR:O | 13:YC:442[A]:THR:HA | 2.03 | 0.59 |
| 13:YA:50[B]:GLU:OE2 | 13:YA:50[B]:GLU:N | 2.33 | 0.59 |
| 13:YA:558[C]:SER:HB3 | 13:YB:551[C]:THR:HG22 | 1.84 | 0.59 |
| 13:YA:397[C]:SER:OG | 13:YB:405[C]:ASP:OD1 | 2.20 | 0.59 |
| 13:YB:538[C]:VAL:HG21 | 13:YC:534[C]:LEU:HD22 | 1.85 | 0.59 |
| 13:YC:25[C]:GLY:HA3 | 13:YC:73[C]:VAL:HG12 | 1.84 | 0.59 |
| 13:YC:50[E]:GLU:OE2 | 13:YC:50[E]:GLU:N | 2.33 | 0.59 |
| 13:YA:60[F]:PRO:CD | 13:YC:61[F]:ILE:HG12 | 2.33 | 0.59 |
| 11:BF:178:ASN:N | 14:YD:217[C]:SER:O | 2.33 | 0.59 |
| 14:YD:332[A]:GLN:HB3 | 14:YE:61[A]:HIS:CE1 | 2.37 | 0.59 |
| 14:YE:232[B]:TYR:OH | 14:YE:312[B]:THR:O | 2.21 | 0.59 |
| 14:YE:35[A]:ILE:HA | 14:YE:54[A]:PHE:HB3 | 1.83 | 0.59 |
| 14:YF:232[B]:TYR:OH | 14:YF:312[B]:THR:O | 2.21 | 0.59 |
| 14:YF:35[E]:ILE:HA | 14:YF:54[E]:PHE:HB3 | 1.83 | 0.59 |
| 14:YF:84[C]:LYS:NZ | 14:YF:317[C]:ASN:OD1 | 2.36 | 0.59 |
| 1:A:17:ILE:HG22 | 1:A:19:GLU:H | 1.67 | 0.59 |
| 1:A:441:ILE:HD11 | 1:A:644:ASN:ND2 | 2.17 | 0.59 |
| 5:AC:426:ASP:O | 5:AC:479:LYS:NZ | 2.36 | 0.59 |
| 5:AD:362:GLU:HB2 | 5:AD:367:GLU:OE1 | 2.03 | 0.59 |
| 7:AI:220:SER:OG | 7:AI:226:GLY:O | 2.20 | 0.59 |
| 7:AJ:509:GLY:HA3 | 7:BA:441:GLN:NE2 | 2.17 | 0.59 |
| 7:AJ:73:THR:HG23 | 7:AJ:74:LYS:H | 1.68 | 0.59 |
| 1:B:209:TRP:O | 1:B:212:LYS:N | 2.35 | 0.59 |
| 1:B:543:THR:HB | 1:B:552:LYS:O | 2.03 | 0.59 |
| 8:BB:89:GLN:HB3 | 8:BB:134:PRO:HG2 | 1.85 | 0.59 |
| 1:BI:543:THR:HB | 1:BI:552:LYS:O | 2.03 | 0.59 |
| 2:C:589:LYS:HB3 | 2:C:592:GLY:O | 2.01 | 0.59 |
| 2:C:977:ILE:HD12 | 2:C:981:GLN:HA | 1.85 | 0.59 |
| 5:CF:426:ASP:O | 5:CF:479:LYS:NZ | 2.36 | 0.59 |
| 5:CF:535:THR:O | 5:CH:576:THR:N | 2.32 | 0.59 |
| 5:CF:472:TYR:HB3 | 5:CG:418:GLY:C | 2.23 | 0.59 |
| 6:CI:58:ASP:OD1 | 6:CJ:164:GLN:NE2 | 2.34 | 0.59 |
| 7:DC:99:ARG:HH12 | 7:DC:101:SER:HB3 | 1.67 | 0.59 |
| 7:DC:513:ARG:O | 7:DD:441:GLN:N | 2.23 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DC:73:THR:HG23 | 7:DC:74:LYS:H | 1.68 | 0.59 |
| 10:DH:332:LEU:HD21 | 10:DH:340:SER:HB3 | 1.85 | 0.59 |
| 10:DH:37:GLN:OE1 | 10:DH:37:GLN:N | 2.36 | 0.59 |
| 1:EA:17:ILE:HG22 | 1:EA:19:GLU:H | 1.67 | 0.59 |
| 2:EC:981:GLN:HG2 | 2:EC:982:LEU:N | 2.16 | 0.59 |
| 3:EE:294:LYS:HB2 | 3:EE:297:TYR:CE1 | 2.38 | 0.59 |
| 7:FE:14:ARG:NH2 | 7:FF:19:ASP:OD2 | 2.34 | 0.59 |
| 7:FF:73:THR:HG23 | 7:FF:74:LYS:H | 1.68 | 0.59 |
| 7:FF:193:LEU:HD21 | 7:FG:207:GLY:HA2 | 1.82 | 0.59 |
| 8:FH:89:GLN:HB3 | 8:FH:134:PRO:HG2 | 1.85 | 0.59 |
| 1:GD:116:ASP:OD1 | 1:GD:117:ALA:N | 2.35 | 0.59 |
| 1:GE:455:PHE:CD2 | 1:GE:456:ASN:HB2 | 2.38 | 0.59 |
| 1:GE:543:THR:HB | 1:GE:552:LYS:O | 2.03 | 0.59 |
| 4:GI:239:ARG:HD2 | 4:GI:249:ILE:HD12 | 1.85 | 0.59 |
| 5:HB:322:GLY:N | 5:HB:358:VAL:O | 2.36 | 0.59 |
| 5:HB:557:TYR:HB2 | 5:HB:559:PRO:HD2 | 1.85 | 0.59 |
| 5:HB:472:TYR:HB3 | 5:HC:418:GLY:C | 2.23 | 0.59 |
| 5:HD:331:CYS:HA | 5:HD:349:TRP:HZ2 | 1.67 | 0.59 |
| 7:HJ:525:VAL:HG23 | 7:HJ:526:LYS:HG2 | 1.84 | 0.59 |
| 5:J:200:LEU:HD22 | 7:P:2:SER:HA | 1.85 | 0.59 |
| 6:M:95:THR:N | 6:M:174:TYR:O | 2.34 | 0.59 |
| 8:S:23:VAL:HB | 8:S:113:VAL:HG23 | 1.84 | 0.59 |
| 1:Y:543:THR:HB | 1:Y:552:LYS:O | 2.03 | 0.59 |
| 1:GD:526:PRO:HB3 | 13:YA:254[B]:ARG:HD3 | 1.84 | 0.59 |
| 13:YA:554[B]:MET:HE2 | 13:YB:550[B]:TRP:CD1 | 2.38 | 0.59 |
| 13:YA:61[F]:ILE:HG22 | 13:YB:76[F]:PRO:HA | 1.84 | 0.59 |
| 13:YB:320[D]:THR:HB | 13:YB:324[D]:ALA:HB2 | 1.84 | 0.59 |
| 13:YB:387[C]:TYR:CZ | 13:YB:388[C]:PRO:HB3 | 2.38 | 0.59 |
| 13:YB:76[A]:PRO:HB2 | 13:YB:98[A]:GLY:N | 2.18 | 0.59 |
| 13:YA:438[B]:LEU:HD22 | 13:YC:442[B]:THR:HG21 | 1.83 | 0.59 |
| 14:YD:70[E]:ILE:HG21 | 14:YD:109[E]:LEU:HD21 | 1.85 | 0.59 |
| 14:YD:35[C]:ILE:HA | 14:YD:54[C]:PHE:HB3 | 1.83 | 0.59 |
| 14:YD:84[C]:LYS:NZ | 14:YD:317[C]:ASN:OD1 | 2.36 | 0.59 |
| 13:YB:47[E]:ILE:HG12 | 14:YE:123[E]:PRO:HD3 | 1.84 | 0.59 |
| 14:YE:84[E]:LYS:NZ | 14:YE:317[E]:ASN:OD1 | 2.36 | 0.59 |
| 14:YF:35[F]:ILE:HA | 14:YF:54[F]:PHE:HB3 | 1.83 | 0.59 |
| 14:YF:84[B]:LYS:NZ | 14:YF:317[B]:ASN:OD1 | 2.35 | 0.59 |
| 2:Z:1006:ASP:OD1 | 2:Z:1007:LEU:N | 2.35 | 0.59 |
| 4:AA:275:ALA:O | 4:AB:282:GLN:NE2 | 2.36 | 0.59 |
| 5:AC:557:TYR:HB2 | 5:AC:559:PRO:HD2 | 1.85 | 0.59 |
| 5:AD:206:PHE:CZ | 5:AD:221:GLU:HG2 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:5:ILE:HD11 | 5:AD:22:GLY:HA2 | 1.84 | 0.59 |
| 5:AD:4:ASN:OD1 | 5:AD:5:ILE:N | 2.36 | 0.59 |
| 5:AD:316:ILE:HG23 | 5:AE:315:GLY:HA3 | 1.85 | 0.59 |
| 5:AD:36:GLU:HG3 | 5:AE:43:PRO:HG2 | 1.84 | 0.59 |
| 7:AJ:233:GLN:HE21 | 7:AJ:237:ASN:ND2 | 2.01 | 0.59 |
| 1:B:646:LEU:O | 2:GF:111:GLN:NE2 | 2.35 | 0.59 |
| 7:BA:132:ARG:NH1 | 7:BA:139:ASN:O | 2.36 | 0.59 |
| 8:BB:38:ALA:HB3 | 8:BB:72:THR:HG22 | 1.85 | 0.59 |
| 1:BH:525:ASN:O | 1:BH:528:THR:OG1 | 2.11 | 0.59 |
| 1:BH:77:GLU:OE2 | 1:BH:88:SER:HB2 | 2.03 | 0.59 |
| 1:BI:440:ILE:HG22 | 1:BI:471:ALA:HB3 | 1.84 | 0.59 |
| 2:BJ:1013:LYS:HE3 | 2:BJ:1022:PRO:HG3 | 1.85 | 0.59 |
| 2:BJ:103:PHE:HZ | 2:BJ:626:GLN:O | 1.85 | 0.59 |
| 2:BJ:246:TYR:HE1 | 2:BJ:255:TYR:HD1 | 1.51 | 0.59 |
| 2:BJ:555:ARG:HG3 | 2:BJ:557:VAL:H | 1.68 | 0.59 |
| 1:B:214:MET:N | 2:C:733:ASP:OD2 | 2.34 | 0.59 |
| 3:CA:294:LYS:HB2 | 3:CA:297:TYR:CZ | 2.38 | 0.59 |
| 4:CC:239:ARG:HD2 | 4:CC:249:ILE:HD12 | 1.85 | 0.59 |
| 5:CG:253:GLN:HE22 | 5:CH:249:ASP:HB3 | 1.68 | 0.59 |
| 5:CH:290:SER:HB2 | 5:CH:370:HIS:HA | 1.84 | 0.59 |
| 7:DD:132:ARG:NH1 | 7:DD:139:ASN:O | 2.36 | 0.59 |
| 7:DC:509:GLY:HA3 | 7:DD:441:GLN:NE2 | 2.17 | 0.59 |
| 8:DE:23:VAL:HB | 8:DE:113:VAL:HG23 | 1.84 | 0.59 |
| 1:EB:208:ASN:HB3 | 1:EB:224:TYR:CE1 | 2.38 | 0.59 |
| 1:EB:455:PHE:CD2 | 1:EB:456:ASN:HB2 | 2.38 | 0.59 |
| 2:EC:1012:LEU:HD13 | 2:EC:1027:GLN:NE2 | 2.18 | 0.59 |
| 2:EC:246:TYR:HE1 | 2:EC:255:TYR:HD1 | 1.51 | 0.59 |
| 2:EC:304:VAL:HG13 | 2:EC:327:ARG:NH1 | 2.16 | 0.59 |
| 2:EC:946:SER:O | 2:EC:947:VAL:HG22 | 2.02 | 0.59 |
| 3:ED:95:TRP:CH2 | 3:ED:169:PRO:HD3 | 2.38 | 0.59 |
| 5:EI:407:TYR:OH | 5:FA:403:THR:HA | 2.03 | 0.59 |
| 5:EJ:188:VAL:HG23 | 5:EJ:225:LEU:HD22 | 1.85 | 0.59 |
| 4:F:239:ARG:HD2 | 4:F:249:ILE:HD12 | 1.85 | 0.59 |
| 7:FE:340:THR:HG22 | 7:FE:341:ILE:HG12 | 1.85 | 0.59 |
| 7:FE:347:MET:HE3 | 7:FF:347:MET:HB3 | 1.84 | 0.59 |
| 7:FF:513:ARG:O | 7:FG:441:GLN:N | 2.22 | 0.59 |
| 7:FG:77:THR:HG23 | 7:FG:79:ALA:N | 2.17 | 0.59 |
| 3:GG:95:TRP:CH2 | 3:GG:169:PRO:HD3 | 2.38 | 0.59 |
| 3:GH:294:LYS:HB2 | 3:GH:297:TYR:CE1 | 2.38 | 0.59 |
| 5:HB:44:TYR:HD2 | 5:HB:48:ALA:HB2 | 1.68 | 0.59 |
| 5:HC:131:SER:HA | 5:HC:150:GLN:HA | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:216:GLY:H | 5:HC:231:ARG:HB2 | 1.68 | 0.59 |
| 5:HC:4:ASN:OD1 | 5:HC:5:ILE:N | 2.36 | 0.59 |
| 5:I:472:TYR:HB3 | 5:J:418:GLY:C | 2.23 | 0.59 |
| 5:I:426:ASP:O | 5:I:479:LYS:NZ | 2.36 | 0.59 |
| 10:ID:332:LEU:HD21 | 10:ID:340:SER:HB3 | 1.85 | 0.59 |
| 5:J:316:ILE:HG23 | 5:K:315:GLY:HA3 | 1.85 | 0.59 |
| 5:J:62:ALA:HB1 | 5:J:82:PRO:HG3 | 1.85 | 0.59 |
| 5:K:213:GLY:O | 5:K:214:SER:OG | 2.19 | 0.59 |
| 5:K:290:SER:CB | 5:K:370:HIS:HA | 2.33 | 0.59 |
| 7:O:218:SER:O | 7:O:227:VAL:HG22 | 2.02 | 0.59 |
| 12:W:230:TYR:CD2 | 12:IF:126:TYR:HA | 2.38 | 0.59 |
| 12:W:161:SER:HB3 | 12:W:240:ASP:HB3 | 1.85 | 0.59 |
| 1:Y:455:PHE:CD2 | 1:Y:456:ASN:HB2 | 2.38 | 0.59 |
| 1:Y:440:ILE:HG22 | 1:Y:471:ALA:HB3 | 1.84 | 0.59 |
| 13:YA:387[D]:TYR:CZ | 13:YA:388[D]:PRO:HB3 | 2.38 | 0.59 |
| 13:YA:57[B]:VAL:CG1 | 13:YA:76[B]:PRO:HD3 | 2.32 | 0.59 |
| 13:YA:83[F]:TYR:CZ | 13:YC:95[F]:ILE:HD11 | 2.38 | 0.59 |
| 13:YB:538[A]:VAL:HG21 | 13:YC:534[A]:LEU:HD22 | 1.85 | 0.59 |
| 13:YB:538[F]:VAL:HG21 | 13:YC:534[F]:LEU:HD22 | 1.85 | 0.59 |
| 13:YC:320[B]:THR:HB | 13:YC:324[B]:ALA:HB2 | 1.84 | 0.59 |
| 13:YC:65[C]:ALA:N | 13:YC:69[C]:ILE:O | 2.36 | 0.59 |
| 14:YD:84[D]:LYS:NZ | 14:YD:317[D]:ASN:OD1 | 2.36 | 0.59 |
| 14:YE:70[E]:ILE:HG21 | 14:YE:109[E]:LEU:HD21 | 1.85 | 0.59 |
| 14:YE:35[B]:ILE:HA | 14:YE:54[B]:PHE:HB3 | 1.83 | 0.59 |
| 2:Z:103:PHE:HZ | 2:Z:626:GLN:O | 1.85 | 0.59 |
| 5:AD:176:ASP:HA | 5:AD:231:ARG:HA | 1.84 | 0.58 |
| 5:AD:310:GLU:HB2 | 5:AD:384:THR:HB | 1.84 | 0.58 |
| 7:AI:101:SER:OG | 7:AI:106:ALA:N | 2.36 | 0.58 |
| 7:AI:473:LYS:HB3 | 7:AJ:473:LYS:HD2 | 1.84 | 0.58 |
| 1:B:206:TRP:CD1 | 1:B:222:THR:HB | 2.38 | 0.58 |
| 1:B:330:THR:O | 1:B:333:ARG:HG2 | 2.03 | 0.58 |
| 1:BI:102:SER:N | 1:BI:194:ARG:HH12 | 2.00 | 0.58 |
| 1:BI:200:TYR:HB2 | 1:BI:269:VAL:CG1 | 2.33 | 0.58 |
| 2:BJ:39:ALA:HB1 | 2:BJ:54:TYR:HE1 | 1.68 | 0.58 |
| 2:C:182:GLN:O | 2:C:210:LYS:NZ | 2.33 | 0.58 |
| 2:C:39:ALA:HB1 | 2:C:54:TYR:HE1 | 1.68 | 0.58 |
| 4:CC:43:GLY:O | 4:CC:68:GLN:NE2 | 2.32 | 0.58 |
| 4:CD:43:GLY:O | 4:CD:68:GLN:NE2 | 2.32 | 0.58 |
| 7:DD:29:ILE:O | 7:DD:30:THR:OG1 | 2.19 | 0.58 |
| 1:EA:77:GLU:OE2 | 1:EA:88:SER:HB2 | 2.03 | 0.58 |
| 4:EG:43:GLY:O | 4:EG:68:GLN:NE2 | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:150:GLN:HB2 | 5:EJ:152:ASP:HB3 | 1.84 | 0.58 |
| 5:FA:507:ASP:OD1 | 5:FA:511:ASN:N | 2.25 | 0.58 |
| 5:FA:86:VAL:HG22 | 5:FA:87:ASN:H | 1.67 | 0.58 |
| 4:G:239:ARG:HD2 | 4:G:249:ILE:HD12 | 1.85 | 0.58 |
| 2:GF:775:ASP:O | 2:GF:776:SER:OG | 2.20 | 0.58 |
| 3:GG:294:LYS:HB2 | 3:GG:297:TYR:CZ | 2.38 | 0.58 |
| 4:H:40:ASN:HB3 | 4:H:45:GLN:HG2 | 1.85 | 0.58 |
| 4:HA:239:ARG:HD2 | 4:HA:249:ILE:HD12 | 1.85 | 0.58 |
| 5:HC:310:GLU:HB2 | 5:HC:384:THR:HB | 1.84 | 0.58 |
| 5:HD:92:VAL:HG12 | 5:HD:136:VAL:HG12 | 1.85 | 0.58 |
| 7:HI:211:SER:H | 7:HI:214:THR:HG1 | 1.50 | 0.58 |
| 7:HI:360:ARG:NH1 | 7:HI:525:VAL:HG21 | 2.18 | 0.58 |
| 7:HJ:29:ILE:O | 7:HJ:30:THR:OG1 | 2.19 | 0.58 |
| 7:HI:509:GLY:HA3 | 7:HJ:441:GLN:NE2 | 2.17 | 0.58 |
| 5:I:117:ILE:HA | 5:I:143:TRP:HB2 | 1.85 | 0.58 |
| 12:GC:213:ALA:HB3 | 12:IF:104:PHE:HZ | 1.67 | 0.58 |
| 5:J:188:VAL:HG23 | 5:J:225:LEU:HD22 | 1.85 | 0.58 |
| 5:J:362:GLU:HB2 | 5:J:367:GLU:OE1 | 2.03 | 0.58 |
| 5:J:356:TYR:HE1 | 6:L:4:LEU:HD13 | 1.68 | 0.58 |
| 7:O:101:SER:OG | 7:O:106:ALA:N | 2.36 | 0.58 |
| 7:P:147:LEU:HB2 | 7:P:148:PRO:HD3 | 1.84 | 0.58 |
| 7:P:97:LEU:HB3 | 7:Q:95:TYR:HB3 | 1.85 | 0.58 |
| 7:Q:365:GLY:O | 7:Q:392:LEU:N | 2.25 | 0.58 |
| 1:Y:208:ASN:HB3 | 1:Y:224:TYR:CE1 | 2.38 | 0.58 |
| 13:YA:387[E]:TYR:CZ | 13:YA:388[E]:PRO:HB3 | 2.37 | 0.58 |
| 13:YA:50[E]:GLU:OE2 | 13:YA:50[E]:GLU:N | 2.33 | 0.58 |
| 13:YB:179[D]:MET:SD | 13:YB:279[D]:ASN:ND2 | 2.76 | 0.58 |
| 13:YB:61[C]:ILE:HG21 | 13:YC:59[C]:GLN:CA | 2.27 | 0.58 |
| 13:YB:65[B]:ALA:N | 13:YB:69[B]:ILE:O | 2.35 | 0.58 |
| 13:YB:65[C]:ALA:N | 13:YB:69[C]:ILE:O | 2.36 | 0.58 |
| 13:YB:434[B]:THR:HG21 | 13:YC:430[B]:ARG:HB3 | 1.85 | 0.58 |
| 13:YC:437[B]:ASN:HB3 | 13:YC:439[B]:TYR:HE1 | 1.66 | 0.58 |
| 13:YB:538[D]:VAL:HG21 | 13:YC:534[D]:LEU:HD22 | 1.85 | 0.58 |
| 13:YA:534[D]:LEU:HB2 | 13:YC:538[D]:VAL:HG11 | 1.84 | 0.58 |
| 13:YC:76[D]:PRO:HB2 | 13:YC:98[D]:GLY:N | 2.18 | 0.58 |
| 14:YD:46[F]:GLY:HA3 | 14:YD:174[F]:ARG:HH22 | 1.67 | 0.58 |
| 14:YD:232[C]:TYR:OH | 14:YD:312[C]:THR:O | 2.21 | 0.58 |
| 14:YD:35[D]:ILE:HA | 14:YD:54[D]:PHE:HB3 | 1.83 | 0.58 |
| 14:YD:70[F]:ILE:HG21 | 14:YD:109[F]:LEU:HD21 | 1.85 | 0.58 |
| 14:YD:84[F]:LYS:NZ | 14:YD:317[F]:ASN:OD1 | 2.36 | 0.58 |
| 14:YE:70[C]:ILE:HG21 | 14:YE:109[C]:LEU:HD21 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:GB:178:ASN:N | 14:YE:217[C]:SER:O | 2.34 | 0.58 |
| 14:YF:125[E]:PHE:CE2 | 14:YF:134[E]:GLU:HG3 | 2.30 | 0.58 |
| 14:YF:41[A]:ARG:HG2 | 14:YF:343[A]:ILE:HG12 | 1.84 | 0.58 |
| 1:A:53:LEU:O | 1:A:53:LEU:HD12 | 2.03 | 0.58 |
| 4:AA:46:ARG:NH2 | 4:AA:66:TYR:OH | 2.36 | 0.58 |
| 5:AC:367:GLU:N | 5:AC:367:GLU:OE1 | 2.36 | 0.58 |
| 5:AC:44:TYR:HD2 | 5:AC:48:ALA:HB2 | 1.68 | 0.58 |
| 5:AC:520:GLY:O | 5:AE:591:PRO:HA | 2.03 | 0.58 |
| 5:AD:188:VAL:HG23 | 5:AD:225:LEU:HD22 | 1.85 | 0.58 |
| 5:AE:92:VAL:HG12 | 5:AE:136:VAL:HG12 | 1.85 | 0.58 |
| 7:AJ:97:LEU:HB3 | 7:BA:95:TYR:HB3 | 1.85 | 0.58 |
| 1:B:281:ASN:HA | 1:B:313:ALA:HB3 | 1.84 | 0.58 |
| 12:BG:144:ASN:H | 10:DH:58:TYR:HE1 | 1.50 | 0.58 |
| 1:BH:441:ILE:HD11 | 1:BH:644:ASN:ND2 | 2.17 | 0.58 |
| 1:BH:582:ASN:OD1 | 1:BH:585:GLY:N | 2.27 | 0.58 |
| 3:CB:294:LYS:HB2 | 3:CB:297:TYR:CE1 | 2.38 | 0.58 |
| 4:CC:42:PHE:O | 4:CC:62:HIS:ND1 | 2.27 | 0.58 |
| 5:CG:216:GLY:H | 5:CG:231:ARG:HB2 | 1.68 | 0.58 |
| 5:CG:36:GLU:HG3 | 5:CH:43:PRO:HG2 | 1.84 | 0.58 |
| 7:DB:163:LEU:HB2 | 7:DC:153:GLY:O | 2.03 | 0.58 |
| 7:DC:97:LEU:HB3 | 7:DD:95:TYR:HB3 | 1.85 | 0.58 |
| 8:DE:89:GLN:HB3 | 8:DE:134:PRO:HG2 | 1.85 | 0.58 |
| 8:DF:89:GLN:HB3 | 8:DF:134:PRO:HG2 | 1.85 | 0.58 |
| 1:EA:286:PHE:HB2 | 1:EA:300:ILE:HD11 | 1.84 | 0.58 |
| 1:EA:53:LEU:HD12 | 1:EA:53:LEU:O | 2.03 | 0.58 |
| 1:EB:440:ILE:HD11 | 1:EB:653:ILE:HG12 | 1.85 | 0.58 |
| 1:EB:440:ILE:HG22 | 1:EB:471:ALA:HB3 | 1.84 | 0.58 |
| 5:EJ:5:ILE:HD11 | 5:EJ:22:GLY:HA2 | 1.84 | 0.58 |
| 7:FE:20:PRO:CD | 7:FE:29:ILE:HG21 | 2.33 | 0.58 |
| 7:FE:310:ASN:HA | 7:FF:316:THR:HB | 1.84 | 0.58 |
| 7:FF:118:PRO:O | 7:FF:122:THR:N | 2.37 | 0.58 |
| 7:FF:360:ARG:NH1 | 7:FF:525:VAL:HG21 | 2.18 | 0.58 |
| 7:FG:132:ARG:NH1 | 7:FG:139:ASN:O | 2.36 | 0.58 |
| 7:FG:418:ASP:OD1 | 7:FG:422:LYS:N | 2.28 | 0.58 |
| 10:GA:332:LEU:HD21 | 10:GA:340:SER:HB3 | 1.85 | 0.58 |
| 1:GD:145:PHE:HZ | 1:GD:286:PHE:HE1 | 1.51 | 0.58 |
| 1:GE:206:TRP:CD1 | 1:GE:222:THR:HB | 2.38 | 0.58 |
| 1:GE:281:ASN:HA | 1:GE:313:ALA:HB3 | 1.84 | 0.58 |
| 1:GE:524:VAL:HG12 | 1:GE:527:ASP:H | 1.68 | 0.58 |
| 3:GG:9:ARG:HD2 | 3:GH:60:TYR:HD1 | 1.67 | 0.58 |
| 4:H:239:ARG:HD2 | 4:H:249:ILE:HD12 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:42:PHE:O | 4:H:62:HIS:ND1 | 2.27 | 0.58 |
| 4:GI:201:LYS:NZ | 4:HA:218:GLU:OE1 | 2.27 | 0.58 |
| 5:HB:367:GLU:OE1 | 5:HB:367:GLU:N | 2.36 | 0.58 |
| 5:HC:188:VAL:HG23 | 5:HC:225:LEU:HD22 | 1.85 | 0.58 |
| 7:HH:162:PRO:HB2 | 7:HI:150:ALA:HA | 1.85 | 0.58 |
| 7:HI:99:ARG:HH12 | 7:HI:101:SER:HB3 | 1.66 | 0.58 |
| 7:HH:422:LYS:HB3 | 7:HI:504:ARG:HA | 1.85 | 0.58 |
| 7:HJ:20:PRO:HB3 | 7:HJ:29:ILE:HG13 | 1.85 | 0.58 |
| 5:I:322:GLY:N | 5:I:358:VAL:O | 2.36 | 0.58 |
| 8:IA:38:ALA:HB3 | 8:IA:72:THR:HG22 | 1.85 | 0.58 |
| 6:M:57:ASN:HB2 | 6:N:164:GLN:NE2 | 2.18 | 0.58 |
| 7:P:211:SER:N | 7:P:214:THR:OG1 | 2.28 | 0.58 |
| 7:O:473:LYS:HB3 | 7:P:473:LYS:HD2 | 1.85 | 0.58 |
| 13:YA:169[A]:ASP:HB2 | 13:YA:343[A]:VAL:HB | 1.85 | 0.58 |
| 13:YA:87[B]:LEU:HD21 | 13:YA:95[B]:ILE:HG23 | 1.85 | 0.58 |
| 13:YB:179[B]:MET:SD | 13:YB:279[B]:ASN:ND2 | 2.75 | 0.58 |
| 13:YB:387[F]:TYR:CZ | 13:YB:388[F]:PRO:HB3 | 2.38 | 0.58 |
| 13:YB:538[B]:VAL:HG21 | 13:YC:534[B]:LEU:HD22 | 1.85 | 0.58 |
| 13:YB:65[F]:ALA:N | 13:YB:69[F]:ILE:O | 2.36 | 0.58 |
| 13:YA:61[A]:ILE:HD11 | 13:YB:72[A]:SER:O | 2.03 | 0.58 |
| 13:YC:17[B]:ASP:OD1 | 13:YC:19[B]:MET:N | 2.36 | 0.58 |
| 13:YC:17[E]:ASP:OD1 | 13:YC:19[E]:MET:N | 2.36 | 0.58 |
| 13:YC:387[C]:TYR:CZ | 13:YC:388[C]:PRO:HB3 | 2.38 | 0.58 |
| 13:YC:76[A]:PRO:HB2 | 13:YC:98[A]:GLY:N | 2.18 | 0.58 |
| 14:YD:125[C]:PHE:CE2 | 14:YD:134[C]:GLU:HG3 | 2.30 | 0.58 |
| 14:YE:125[A]:PHE:CE2 | 14:YE:134[A]:GLU:HG3 | 2.30 | 0.58 |
| 11:BF:190:LYS:HE3 | 14:YE:24[B]:SER:O | 2.03 | 0.58 |
| 14:YE:232[E]:TYR:OH | 14:YE:312[E]:THR:O | 2.21 | 0.58 |
| 14:YF:70[C]:ILE:HG21 | 14:YF:109[C]:LEU:HD21 | 1.85 | 0.58 |
| 14:YF:70[E]:ILE:HG21 | 14:YF:109[E]:LEU:HD21 | 1.85 | 0.58 |
| 14:YF:46[B]:GLY:HA3 | 14:YF:174[B]:ARG:HH22 | 1.67 | 0.58 |
| 14:YF:84[E]:LYS:NZ | 14:YF:317[E]:ASN:OD1 | 2.36 | 0.58 |
| 2:Z:1013:LYS:HE3 | 2:Z:1022:PRO:HG3 | 1.85 | 0.58 |
| 2:Z:1012:LEU:HD13 | 2:Z:1027:GLN:NE2 | 2.18 | 0.58 |
| 2:Z:589:LYS:HB3 | 2:Z:592:GLY:O | 2.01 | 0.58 |
| 13:YC:572[A]:ILE:HD12 | 15:ZA:94[A]:VAL:HG22 | 1.83 | 0.58 |
| 1:A:286:PHE:HB2 | 1:A:300:ILE:HD11 | 1.84 | 0.58 |
| 5:AC:187:ASN:HB2 | 5:AC:254:TRP:CZ2 | 2.39 | 0.58 |
| 5:AC:322:GLY:N | 5:AC:358:VAL:O | 2.36 | 0.58 |
| 5:AC:154:ILE:HG12 | 5:AD:153:LYS:HZ2 | 1.68 | 0.58 |
| 5:AE:328:LEU:HD12 | 5:AE:330:HIS:CD2 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:43:PRO:HG3 | 5:AE:33:LEU:HA | 1.85 | 0.58 |
| 5:AD:542:LEU:HD11 | 5:AE:569:TYR:CE2 | 2.39 | 0.58 |
| 5:AC:517:GLY:N | 5:AE:594:THR:OG1 | 2.36 | 0.58 |
| 7:AJ:99:ARG:HD2 | 7:BA:95:TYR:HE1 | 1.66 | 0.58 |
| 1:B:87:SER:OG | 1:B:230:ILE:O | 2.12 | 0.58 |
| 1:BH:145:PHE:HZ | 1:BH:286:PHE:HE1 | 1.51 | 0.58 |
| 1:BH:53:LEU:HD12 | 1:BH:53:LEU:O | 2.03 | 0.58 |
| 1:BI:174:ARG:NH2 | 1:BI:269:VAL:HG21 | 2.18 | 0.58 |
| 2:BJ:529:SER:O | 2:BJ:531:ARG:HG3 | 2.04 | 0.58 |
| 2:BJ:781:LEU:HB2 | 2:BJ:798:ILE:HD11 | 1.86 | 0.58 |
| 3:CA:9:ARG:HD2 | 3:CB:60:TYR:HD1 | 1.68 | 0.58 |
| 4:CD:40:ASN:HB3 | 4:CD:45:GLN:HG2 | 1.85 | 0.58 |
| 5:CF:183:GLY:HA2 | 5:CF:307:ASN:HD22 | 1.68 | 0.58 |
| 5:CH:371:PHE:CZ | 5:CH:373:SER:HB3 | 2.38 | 0.58 |
| 5:CF:517:GLY:N | 5:CH:594:THR:OG1 | 2.37 | 0.58 |
| 3:D:261:ALA:O | 3:D:266:ASN:ND2 | 2.30 | 0.58 |
| 6:CJ:57:ASN:HB2 | 6:DA:164:GLN:NE2 | 2.18 | 0.58 |
| 7:DC:233:GLN:HE21 | 7:DC:237:ASN:ND2 | 2.01 | 0.58 |
| 7:DC:334:GLN:HG3 | 7:DC:337:ILE:HD12 | 1.84 | 0.58 |
| 7:DC:40:SER:O | 7:DD:24:ASN:ND2 | 2.37 | 0.58 |
| 7:DC:422:LYS:NZ | 7:DD:498:SER:O | 2.36 | 0.58 |
| 8:DE:38:ALA:HB3 | 8:DE:72:THR:HG22 | 1.85 | 0.58 |
| 3:E:294:LYS:HB2 | 3:E:297:TYR:CE1 | 2.38 | 0.58 |
| 1:EB:200:TYR:HB2 | 1:EB:269:VAL:CG1 | 2.33 | 0.58 |
| 1:EB:543:THR:HB | 1:EB:552:LYS:O | 2.03 | 0.58 |
| 2:EC:49:LEU:HB3 | 2:EC:50:PRO:HD3 | 1.85 | 0.58 |
| 4:EF:42:PHE:O | 4:EF:62:HIS:ND1 | 2.27 | 0.58 |
| 5:EI:146:VAL:HG23 | 5:EJ:153:LYS:HB2 | 1.84 | 0.58 |
| 5:EJ:176:ASP:HA | 5:EJ:231:ARG:HA | 1.84 | 0.58 |
| 7:FF:40:SER:O | 7:FG:24:ASN:ND2 | 2.35 | 0.58 |
| 8:FH:23:VAL:HB | 8:FH:113:VAL:HG23 | 1.84 | 0.58 |
| 8:FI:23:VAL:HB | 8:FI:113:VAL:HG23 | 1.84 | 0.58 |
| 1:GD:338:ARG:NH2 | 1:GE:340:VAL:O | 2.36 | 0.58 |
| 2:GF:39:ALA:HB1 | 2:GF:54:TYR:HE1 | 1.68 | 0.58 |
| 5:HB:183:GLY:HA2 | 5:HB:307:ASN:HD22 | 1.68 | 0.58 |
| 5:HB:43:PRO:HG3 | 5:HD:33:LEU:HA | 1.86 | 0.58 |
| 6:HE:12:SER:CB | 6:HG:6:ASN:HB3 | 2.34 | 0.58 |
| 5:I:139:ALA:HB3 | 5:J:99:PHE:HB3 | 1.85 | 0.58 |
| 8:IA:23:VAL:HB | 8:IA:113:VAL:HG23 | 1.84 | 0.58 |
| 8:IA:68:ASP:OD1 | 8:IA:69:TRP:N | 2.36 | 0.58 |
| 12:IF:111:ILE:O | 12:IF:115:ASN:N | 2.28 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:IF:161:SER:HB3 | 12:IF:240:ASP:HB3 | 1.85 | 0.58 |
| 2:C:992:PRO:HB3 | 5:K:19:LEU:HB3 | 1.86 | 0.58 |
| 6:L:13:ARG:NH1 | 6:N:17:PHE:O | 2.27 | 0.58 |
| 7:P:73:THR:HG23 | 7:P:74:LYS:H | 1.68 | 0.58 |
| 7:Q:12:GLU:HB3 | 7:Q:15:TYR:HB3 | 1.84 | 0.58 |
| 7:O:134:SER:HB2 | 7:Q:143:LYS:HA | 1.85 | 0.58 |
| 10:U:288:SER:OG | 10:U:289:ASN:N | 2.36 | 0.58 |
| 11:V:57:GLU:N | 11:V:57:GLU:OE1 | 2.25 | 0.58 |
| 1:Y:200:TYR:HB2 | 1:Y:269:VAL:CG1 | 2.33 | 0.58 |
| 13:YA:17[B]:ASP:OD1 | 13:YA:19[B]:MET:N | 2.36 | 0.58 |
| 13:YA:434[B]:THR:O | 13:YC:442[B]:THR:HA | 2.03 | 0.58 |
| 13:YA:534[B]:LEU:HB2 | 13:YC:538[B]:VAL:HG11 | 1.84 | 0.58 |
| 13:YA:61[B]:ILE:HA | 13:YB:76[B]:PRO:C | 2.24 | 0.58 |
| 13:YA:61[F]:ILE:HG13 | 13:YA:62[F]:THR:N | 2.17 | 0.58 |
| 13:YB:17[A]:ASP:OD1 | 13:YB:19[A]:MET:N | 2.37 | 0.58 |
| 13:YB:387[E]:TYR:CZ | 13:YB:388[E]:PRO:HB3 | 2.37 | 0.58 |
| 13:YB:416[C]:HIS:CD2 | 13:YB:418[C]:THR:H | 2.21 | 0.58 |
| 13:YB:57[D]:VAL:CG1 | 13:YB:76[D]:PRO:HD3 | 2.34 | 0.58 |
| 13:YB:76[D]:PRO:HG3 | 13:YB:96[D]:VAL:HB | 1.83 | 0.58 |
| 13:YC:169[D]:ASP:HB2 | 13:YC:343[D]:VAL:HB | 1.85 | 0.58 |
| 13:YC:65[B]:ALA:N | 13:YC:69[B]:ILE:O | 2.35 | 0.58 |
| 14:YD:70[C]:ILE:HG21 | 14:YD:109[C]:LEU:HD21 | 1.85 | 0.58 |
| 14:YD:232[A]:TYR:OH | 14:YD:312[A]:THR:O | 2.21 | 0.58 |
| 14:YD:332[F]:GLN:HB3 | 14:YE:61[F]:HIS:CE1 | 2.38 | 0.58 |
| 14:YE:46[F]:GLY:HA3 | 14:YE:174[F]:ARG:HH22 | 1.67 | 0.58 |
| 14:YF:70[F]:ILE:HG21 | 14:YF:109[F]:LEU:HD21 | 1.85 | 0.58 |
| 2:Z:403:ILE:HG21 | 2:Z:417:PHE:HB3 | 1.83 | 0.58 |
| 2:Z:561:TRP:CZ3 | 2:Z:566:CYS:HB2 | 2.38 | 0.58 |
| 2:Z:946:SER:O | 2:Z:947:VAL:HG22 | 2.02 | 0.58 |
| 13:YA:572[E]:ILE:O | 15:ZA:68[E]:TYR:HB2 | 2.03 | 0.58 |
| 13:YA:572[F]:ILE:O | 15:ZA:68[F]:TYR:HB2 | 2.03 | 0.58 |
| 1:A:209:TRP:HD1 | 1:A:225:TYR:HE1 | 1.51 | 0.58 |
| 1:A:87:SER:OG | 1:A:230:ILE:O | 2.21 | 0.58 |
| 5:AC:154:ILE:HB | 5:AE:156:SER:HB2 | 1.85 | 0.58 |
| 5:AE:507:ASP:OD1 | 5:AE:511:ASN:N | 2.25 | 0.58 |
| 1:B:440:ILE:HD11 | 1:B:653:ILE:HG12 | 1.85 | 0.58 |
| 1:BH:423:THR:O | 1:BH:476:ILE:N | 2.35 | 0.58 |
| 1:BI:206:TRP:CD1 | 1:BI:222:THR:HB | 2.38 | 0.58 |
| 2:BJ:946:SER:O | 2:BJ:947:VAL:HG22 | 2.02 | 0.58 |
| 2:C:103:PHE:HZ | 2:C:626:GLN:O | 1.85 | 0.58 |
| 5:CF:557:TYR:HB2 | 5:CF:559:PRO:HD2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:5:ILE:HD11 | 5:CG:22:GLY:HA2 | 1.84 | 0.58 |
| 5:CG:72:THR:HG22 | 5:CG:77:VAL:HG22 | 1.85 | 0.58 |
| 7:DD:453:GLU:OE2 | 7:DD:471:THR:N | 2.29 | 0.58 |
| 8:DF:38:ALA:HB3 | 8:DF:72:THR:HG22 | 1.85 | 0.58 |
| 2:EC:189:ARG:HG2 | 2:EC:204:ARG:HH12 | 1.69 | 0.58 |
| 4:EF:40:ASN:HB3 | 4:EF:45:GLN:HG2 | 1.85 | 0.58 |
| 4:EG:40:ASN:HB3 | 4:EG:45:GLN:HG2 | 1.85 | 0.58 |
| 5:EI:44:TYR:HD2 | 5:EI:48:ALA:HB2 | 1.68 | 0.58 |
| 5:EJ:206:PHE:CZ | 5:EJ:221:GLU:HG2 | 2.38 | 0.58 |
| 5:EJ:263:ILE:HG22 | 5:EJ:381:ILE:HB | 1.86 | 0.58 |
| 5:EJ:72:THR:HG22 | 5:EJ:77:VAL:HG22 | 1.85 | 0.58 |
| 4:F:171:LYS:HB2 | 4:G:165:GLU:HB3 | 1.85 | 0.58 |
| 5:EI:43:PRO:HG2 | 5:FA:36:GLU:HG3 | 1.83 | 0.58 |
| 7:FE:375:TYR:HE2 | 7:FE:390:PRO:HB2 | 1.69 | 0.58 |
| 7:FF:44:VAL:HG21 | 7:FG:25:PHE:HB3 | 1.85 | 0.58 |
| 7:FG:296:ILE:HG22 | 7:FG:298:GLY:H | 1.67 | 0.58 |
| 1:GE:440:ILE:HG22 | 1:GE:471:ALA:HB3 | 1.84 | 0.58 |
| 2:GF:561:TRP:CZ3 | 2:GF:566:CYS:HB2 | 2.38 | 0.58 |
| 4:GI:40:ASN:HB3 | 4:GI:45:GLN:HG2 | 1.85 | 0.58 |
| 5:HB:569:TYR:H | 5:HC:550:VAL:HB | 1.68 | 0.58 |
| 5:HC:263:ILE:HG22 | 5:HC:381:ILE:HB | 1.86 | 0.58 |
| 5:HD:213:GLY:O | 5:HD:221:GLU:HB2 | 2.04 | 0.58 |
| 5:HD:359:GLU:HB3 | 5:HD:370:HIS:HB3 | 1.84 | 0.58 |
| 5:HD:371:PHE:CZ | 5:HD:373:SER:HB3 | 2.38 | 0.58 |
| 7:HI:386:ASN:HB2 | 7:HI:387:PRO:HD2 | 1.85 | 0.58 |
| 7:HH:512:THR:HA | 7:HI:442:MET:HA | 1.84 | 0.58 |
| 5:J:5:ILE:HD11 | 5:J:22:GLY:HA2 | 1.84 | 0.58 |
| 5:K:313:PHE:CE2 | 5:K:320:LEU:HD21 | 2.39 | 0.58 |
| 7:O:20:PRO:CD | 7:O:29:ILE:HG21 | 2.33 | 0.58 |
| 7:P:334:GLN:HG3 | 7:P:337:ILE:HD12 | 1.84 | 0.58 |
| 8:S:89:GLN:HB3 | 8:S:134:PRO:HG2 | 1.85 | 0.58 |
| 10:U:37:GLN:OE1 | 10:U:37:GLN:N | 2.36 | 0.58 |
| 1:X:336:GLN:HG3 | 1:X:337:GLN:H | 1.67 | 0.58 |
| 1:Y:281:ASN:HA | 1:Y:313:ALA:HB3 | 1.84 | 0.58 |
| 1:Y:52:ARG:HD3 | 2:Z:657:TYR:HD1 | 1.68 | 0.58 |
| 13:YA:320[D]:THR:HB | 13:YA:324[D]:ALA:HB2 | 1.84 | 0.58 |
| 13:YA:320[F]:THR:HB | 13:YA:324[F]:ALA:HB2 | 1.85 | 0.58 |
| 13:YA:387[B]:TYR:CZ | 13:YA:388[B]:PRO:HB3 | 2.37 | 0.58 |
| 13:YA:558[B]:SER:HB3 | 13:YB:551[B]:THR:HG22 | 1.84 | 0.58 |
| 13:YB:291[B]:LYS:HZ3 | 13:YC:362[B]:ASP:N | 2.01 | 0.58 |
| 13:YB:169[D]:ASP:HB2 | 13:YB:343[D]:VAL:HB | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:82[D]:VAL:HG22 | 13:YB:98[D]:GLY:O | 2.04 | 0.58 |
| 13:YC:169[C]:ASP:HB2 | 13:YC:343[C]:VAL:HB | 1.86 | 0.58 |
| 13:YC:387[E]:TYR:CZ | 13:YC:388[E]:PRO:HB3 | 2.37 | 0.58 |
| 13:YA:534[A]:LEU:HB2 | 13:YC:538[A]:VAL:HG11 | 1.84 | 0.58 |
| 13:YA:59[B]:GLN:HA | 13:YC:61[B]:ILE:HG21 | 1.85 | 0.58 |
| 13:YC:82[A]:VAL:HG22 | 13:YC:98[A]:GLY:O | 2.04 | 0.58 |
| 14:YE:232[F]:TYR:OH | 14:YE:312[F]:THR:O | 2.20 | 0.58 |
| 14:YE:332[C]:GLN:HB3 | 14:YF:61[C]:HIS:CE1 | 2.38 | 0.58 |
| 5:AE:213:GLY:O | 5:AE:221:GLU:HB2 | 2.03 | 0.58 |
| 5:AE:359:GLU:HB3 | 5:AE:370:HIS:HB3 | 1.84 | 0.58 |
| 1:B:455:PHE:CD1 | 1:B:639:LEU:HD12 | 2.35 | 0.58 |
| 8:BC:68:ASP:OD1 | 8:BC:69:TRP:N | 2.36 | 0.58 |
| 12:BG:161:SER:HB3 | 12:BG:240:ASP:HB3 | 1.85 | 0.58 |
| 1:BH:558:PHE:O | 1:BH:586:ARG:HB2 | 2.04 | 0.58 |
| 1:BI:330:THR:O | 1:BI:333:ARG:HG2 | 2.03 | 0.58 |
| 2:BJ:241:SER:HB2 | 2:BJ:313:CYS:SG | 2.44 | 0.58 |
| 2:BJ:340:PRO:HA | 2:BJ:345:TYR:HE1 | 1.67 | 0.58 |
| 2:BJ:901:ASN:OD1 | 3:CB:333:THR:OG1 | 2.21 | 0.58 |
| 2:BJ:963:TYR:CD1 | 2:BJ:964:PRO:HD2 | 2.39 | 0.58 |
| 2:C:168:ILE:HG12 | 2:C:578:PHE:HZ | 1.69 | 0.58 |
| 4:CC:46:ARG:NH2 | 4:CC:66:TYR:OH | 2.36 | 0.58 |
| 5:CG:4:ASN:OD1 | 5:CG:5:ILE:N | 2.36 | 0.58 |
| 5:CH:313:PHE:CE2 | 5:CH:320:LEU:HD21 | 2.39 | 0.58 |
| 7:DB:375:TYR:HE2 | 7:DB:390:PRO:HB2 | 1.69 | 0.58 |
| 1:EA:278:ALA:HB2 | 1:EA:317:GLY:H | 1.67 | 0.58 |
| 2:EC:340:PRO:HA | 2:EC:345:TYR:HE1 | 1.68 | 0.58 |
| 2:EC:39:ALA:HB1 | 2:EC:54:TYR:HE1 | 1.68 | 0.58 |
| 3:ED:46:PRO:HG3 | 3:ED:270:ARG:HH22 | 1.68 | 0.58 |
| 4:EF:131:LYS:N | 4:EF:160:TRP:O | 2.29 | 0.58 |
| 5:EI:183:GLY:HA2 | 5:EI:307:ASN:HD22 | 1.68 | 0.58 |
| 5:EI:426:ASP:O | 5:EI:479:LYS:NZ | 2.36 | 0.58 |
| 2:EC:984:SER:OG | 5:EJ:12:ASP:OD2 | 2.10 | 0.58 |
| 5:EJ:216:GLY:H | 5:EJ:231:ARG:HB2 | 1.68 | 0.58 |
| 5:EJ:62:ALA:HB1 | 5:EJ:82:PRO:HG3 | 1.85 | 0.58 |
| 5:FA:359:GLU:HB3 | 5:FA:370:HIS:HB3 | 1.84 | 0.58 |
| 5:FA:490:TRP:NE1 | 5:FA:515:THR:O | 2.36 | 0.58 |
| 6:FD:100:PRO:O | 6:FD:103:SER:OG | 2.18 | 0.58 |
| 7:FE:162:PRO:HB2 | 7:FF:150:ALA:HA | 1.85 | 0.58 |
| 7:FF:99:ARG:HD2 | 7:FG:95:TYR:HE1 | 1.69 | 0.58 |
| 8:DE:120:ALA:HB3 | 8:FI:99:ILE:O | 2.04 | 0.58 |
| 11:GB:36:PHE:HZ | 11:GB:76:CYS:HG | 1.50 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:286:PHE:HB2 | 1:GD:300:ILE:HD11 | 1.84 | 0.58 |
| 2:GF:360:ASN:C | 2:GF:362:LYS:H | 2.02 | 0.58 |
| 2:GF:578:PHE:CE2 | 2:GF:582:ALA:HB2 | 2.38 | 0.58 |
| 5:HC:285:LEU:HD11 | 5:HC:375:PHE:CB | 2.28 | 0.58 |
| 5:HC:72:THR:HG22 | 5:HC:77:VAL:HG22 | 1.85 | 0.58 |
| 5:HD:398:GLU:N | 5:HD:398:GLU:OE1 | 2.37 | 0.58 |
| 5:HC:590:GLN:HE21 | 5:HD:486:VAL:HG11 | 1.69 | 0.58 |
| 5:I:44:TYR:HD2 | 5:I:48:ALA:HB2 | 1.68 | 0.58 |
| 8:S:104:PRO:HD3 | 8:IA:14:ASP:HB2 | 1.84 | 0.58 |
| 8:IB:23:VAL:HB | 8:IB:113:VAL:HG23 | 1.84 | 0.58 |
| 8:IB:38:ALA:HB3 | 8:IB:72:THR:HG22 | 1.85 | 0.58 |
| 11:IE:190:LYS:HE3 | 14:YF:24[C]:SER:O | 2.03 | 0.58 |
| 5:J:542:LEU:HD11 | 5:K:569:TYR:CE2 | 2.38 | 0.58 |
| 5:K:102:TRP:HE3 | 5:K:131:SER:HB2 | 1.67 | 0.58 |
| 6:L:10:VAL:HA | 6:M:13:ARG:HD2 | 1.84 | 0.58 |
| 7:O:310:ASN:HA | 7:P:316:THR:HB | 1.83 | 0.58 |
| 7:O:340:THR:HG22 | 7:O:341:ILE:HG12 | 1.85 | 0.58 |
| 7:P:360:ARG:NH1 | 7:P:525:VAL:HG21 | 2.18 | 0.58 |
| 5:K:196:ARG:NH1 | 7:P:5:THR:O | 2.36 | 0.58 |
| 10:U:332:LEU:HD21 | 10:U:340:SER:HB3 | 1.85 | 0.58 |
| 11:V:131:TYR:O | 11:V:148:GLY:N | 2.25 | 0.58 |
| 1:X:431:GLU:HG2 | 1:X:435:TRP:CE3 | 2.39 | 0.58 |
| 13:YA:169[C]:ASP:HB2 | 13:YA:343[C]:VAL:HB | 1.86 | 0.58 |
| 13:YA:424[B]:VAL:HA | 13:YA:429[B]:ARG:O | 2.04 | 0.58 |
| 13:YA:76[A]:PRO:HB2 | 13:YA:98[A]:GLY:N | 2.18 | 0.58 |
| 13:YB:291[F]:LYS:HZ3 | 13:YC:362[F]:ASP:N | 2.02 | 0.58 |
| 13:YB:169[A]:ASP:HB2 | 13:YB:343[A]:VAL:HB | 1.85 | 0.58 |
| 13:YB:169[F]:ASP:HB2 | 13:YB:343[F]:VAL:HB | 1.86 | 0.58 |
| 13:YB:416[B]:HIS:CD2 | 13:YB:418[B]:THR:H | 2.22 | 0.58 |
| 13:YB:437[D]:ASN:HB3 | 13:YB:439[D]:TYR:HE1 | 1.67 | 0.58 |
| 13:YA:554[A]:MET:HE2 | 13:YB:550[A]:TRP:CD1 | 2.39 | 0.58 |
| 13:YC:437[C]:ASN:HB3 | 13:YC:439[C]:TYR:HE1 | 1.66 | 0.58 |
| 13:YA:434[F]:THR:O | 13:YC:442[F]:THR:HA | 2.03 | 0.58 |
| 13:YC:57[D]:VAL:CG1 | 13:YC:76[D]:PRO:HD3 | 2.34 | 0.58 |
| 14:YD:46[B]:GLY:HA3 | 14:YD:174[B]:ARG:HH22 | 1.67 | 0.58 |
| 14:YE:46[E]:GLY:HA3 | 14:YE:174[E]:ARG:HH22 | 1.67 | 0.58 |
| 14:YF:232[D]:TYR:OH | 14:YF:312[D]:THR:O | 2.21 | 0.58 |
| 2:Z:168:ILE:HG12 | 2:Z:578:PHE:HZ | 1.69 | 0.58 |
| 1:Y:496:GLU:HG3 | 2:Z:856:ASN:O | 2.04 | 0.58 |
| 1:A:145:PHE:HZ | 1:A:286:PHE:HE1 | 1.52 | 0.58 |
| 5:AC:419:ASP:OD1 | 5:AC:420:VAL:N | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:253:GLN:HE22 | 5:AE:249:ASP:HB3 | 1.69 | 0.58 |
| 5:AD:285:LEU:HD11 | 5:AD:375:PHE:CB | 2.28 | 0.58 |
| 5:AC:139:ALA:HB3 | 5:AD:99:PHE:HB3 | 1.85 | 0.58 |
| 7:AI:163:LEU:HB2 | 7:AJ:153:GLY:O | 2.03 | 0.58 |
| 7:AJ:386:ASN:HB2 | 7:AJ:387:PRO:HD2 | 1.85 | 0.58 |
| 1:BH:336:GLN:HG3 | 1:BH:337:GLN:H | 1.67 | 0.58 |
| 1:BI:524:VAL:HG12 | 1:BI:527:ASP:H | 1.68 | 0.58 |
| 2:C:529:SER:O | 2:C:531:ARG:HG3 | 2.04 | 0.58 |
| 2:C:703:TYR:O | 2:C:706:SER:N | 2.31 | 0.58 |
| 2:C:715:LEU:HG | 2:C:716:ASN:H | 1.67 | 0.58 |
| 4:CD:171:LYS:HB2 | 4:CE:165:GLU:HB3 | 1.86 | 0.58 |
| 5:CF:154:ILE:HG12 | 5:CG:153:LYS:HZ2 | 1.68 | 0.58 |
| 5:CF:285:LEU:HD21 | 5:CF:375:PHE:H | 1.68 | 0.58 |
| 5:CH:213:GLY:O | 5:CH:221:GLU:HB2 | 2.04 | 0.58 |
| 5:CF:43:PRO:HG3 | 5:CH:33:LEU:HA | 1.86 | 0.58 |
| 7:DB:101:SER:OG | 7:DB:106:ALA:N | 2.36 | 0.58 |
| 1:EA:145:PHE:HZ | 1:EA:286:PHE:HE1 | 1.52 | 0.58 |
| 2:EC:241:SER:HB2 | 2:EC:313:CYS:SG | 2.44 | 0.58 |
| 2:EC:338:PHE:HE2 | 2:EC:342:SER:O | 1.87 | 0.58 |
| 2:EC:168:ILE:HG12 | 2:EC:578:PHE:HZ | 1.69 | 0.58 |
| 2:EC:578:PHE:CE2 | 2:EC:582:ALA:HB2 | 2.38 | 0.58 |
| 2:EC:675:LEU:O | 2:EC:681:THR:HB | 2.04 | 0.58 |
| 3:EE:177:GLU:HG3 | 3:EE:180:ILE:HG22 | 1.86 | 0.58 |
| 4:EF:46:ARG:NH2 | 4:EF:66:TYR:OH | 2.36 | 0.58 |
| 4:EH:46:ARG:NH2 | 4:EH:66:TYR:OH | 2.36 | 0.58 |
| 5:EI:557:TYR:HB2 | 5:EI:559:PRO:HD2 | 1.85 | 0.58 |
| 5:EJ:146:VAL:HB | 5:FA:153:LYS:HA | 1.85 | 0.58 |
| 5:FA:290:SER:HB2 | 5:FA:370:HIS:HA | 1.84 | 0.58 |
| 7:FE:12:GLU:HB3 | 7:FE:15:TYR:HB3 | 1.86 | 0.58 |
| 7:FF:386:ASN:HB2 | 7:FF:387:PRO:HD2 | 1.85 | 0.58 |
| 8:FH:68:ASP:OD1 | 8:FH:69:TRP:N | 2.36 | 0.58 |
| 11:GB:131:TYR:O | 11:GB:148:GLY:N | 2.25 | 0.58 |
| 12:GC:111:ILE:O | 12:GC:115:ASN:N | 2.28 | 0.58 |
| 1:GD:502:ASN:N | 1:GD:600:ASP:OD2 | 2.37 | 0.58 |
| 2:GF:529:SER:O | 2:GF:531:ARG:HG3 | 2.04 | 0.58 |
| 2:GF:575:PHE:HB2 | 2:GF:608:VAL:HG22 | 1.85 | 0.58 |
| 4:GJ:239:ARG:HD2 | 4:GJ:249:ILE:HD12 | 1.85 | 0.58 |
| 4:HA:40:ASN:HB3 | 4:HA:45:GLN:HG2 | 1.85 | 0.58 |
| 5:HB:195:HIS:HE2 | 5:HB:236:CYS:HG | 1.50 | 0.58 |
| 5:HC:206:PHE:CG | 5:HC:223:VAL:HA | 2.37 | 0.58 |
| 5:HD:313:PHE:CE2 | 5:HD:320:LEU:HD21 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:318:GLN:HE22 | 6:HF:8:ALA:N | 2.01 | 0.58 |
| 2:GF:654:PRO:HG3 | 9:IC:47:ARG:HD2 | 1.86 | 0.58 |
| 12:IF:216:PHE:CE1 | 12:IF:218:MET:HE3 | 2.38 | 0.58 |
| 5:J:318:GLN:HE22 | 6:L:8:ALA:N | 2.02 | 0.58 |
| 7:O:184:THR:OG1 | 7:O:187:ASP:N | 2.34 | 0.58 |
| 7:P:99:ARG:HH12 | 7:P:101:SER:HB3 | 1.67 | 0.58 |
| 7:P:509:GLY:HA3 | 7:Q:441:GLN:NE2 | 2.18 | 0.58 |
| 12:W:177:TRP:CZ3 | 12:W:220:SER:HB3 | 2.38 | 0.58 |
| 1:Y:455:PHE:CD1 | 1:Y:639:LEU:HD12 | 2.35 | 0.58 |
| 13:YA:387[A]:TYR:CZ | 13:YA:388[A]:PRO:HB3 | 2.38 | 0.58 |
| 13:YA:387[C]:TYR:CZ | 13:YA:388[C]:PRO:HB3 | 2.38 | 0.58 |
| 13:YA:434[D]:THR:O | 13:YC:442[D]:THR:HA | 2.03 | 0.58 |
| 13:YA:82[D]:VAL:HG22 | 13:YA:98[D]:GLY:O | 2.04 | 0.58 |
| 13:YB:179[A]:MET:SD | 13:YB:279[A]:ASN:ND2 | 2.76 | 0.58 |
| 13:YB:17[B]:ASP:OD1 | 13:YB:19[B]:MET:N | 2.36 | 0.58 |
| 13:YB:17[D]:ASP:OD1 | 13:YB:19[D]:MET:N | 2.37 | 0.58 |
| 13:YB:416[D]:HIS:HD2 | 13:YB:418[D]:THR:H | 1.51 | 0.58 |
| 13:YB:567[C]:ILE:HG23 | 13:YC:565[C]:TYR:CE2 | 2.39 | 0.58 |
| 13:YB:567[D]:ILE:HG23 | 13:YC:565[D]:TYR:CE2 | 2.39 | 0.58 |
| 13:YB:57[B]:VAL:CG1 | 13:YB:76[B]:PRO:HD3 | 2.32 | 0.58 |
| 13:YC:17[D]:ASP:OD1 | 13:YC:19[D]:MET:N | 2.37 | 0.58 |
| 13:YB:434[F]:THR:HG21 | 13:YC:430[F]:ARG:HB3 | 1.85 | 0.58 |
| 13:YA:434[E]:THR:O | 13:YC:442[E]:THR:HA | 2.03 | 0.58 |
| 13:YB:538[E]:VAL:HG21 | 13:YC:534[E]:LEU:HD22 | 1.85 | 0.58 |
| 13:YA:534[E]:LEU:HB2 | 13:YC:538[E]:VAL:HG11 | 1.85 | 0.58 |
| 13:YA:555[A]:ALA:O | 13:YC:563[A]:GLY:N | 2.36 | 0.58 |
| 13:YA:555[B]:ALA:O | 13:YC:563[B]:GLY:N | 2.36 | 0.58 |
| 14:YF:232[C]:TYR:OH | 14:YF:312[C]:THR:O | 2.21 | 0.58 |
| 14:YF:70[D]:ILE:HG21 | 14:YF:109[D]:LEU:HD21 | 1.85 | 0.58 |
| 2:Z:555:ARG:HG3 | 2:Z:557:VAL:H | 1.68 | 0.58 |
| 1:A:399:TYR:O | 1:A:400:ASN:HB2 | 2.04 | 0.58 |
| 1:A:431:GLU:HG2 | 1:A:435:TRP:CE3 | 2.39 | 0.58 |
| 1:A:502:ASN:N | 1:A:600:ASP:OD2 | 2.37 | 0.58 |
| 5:AD:334:ALA:O | 5:AD:337:ASP:N | 2.35 | 0.58 |
| 5:AE:102:TRP:HE3 | 5:AE:131:SER:HB2 | 1.67 | 0.58 |
| 5:AE:398:GLU:OE1 | 5:AE:398:GLU:N | 2.37 | 0.58 |
| 5:AE:490:TRP:NE1 | 5:AE:515:THR:O | 2.37 | 0.58 |
| 7:AI:43:GLY:O | 7:AJ:42:ALA:HB3 | 2.04 | 0.58 |
| 1:B:102:SER:N | 1:B:194:ARG:HH12 | 2.00 | 0.58 |
| 1:B:174:ARG:NH2 | 1:B:269:VAL:HG21 | 2.18 | 0.58 |
| 1:B:209:TRP:HE3 | 1:B:212:LYS:HB2 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:200:TYR:HB2 | 1:B:269:VAL:CG1 | 2.33 | 0.58 |
| 1:B:455:PHE:CD2 | 1:B:456:ASN:HB2 | 2.38 | 0.58 |
| 1:BH:544:ASP:HB2 | 1:BH:576:ASP:CG | 2.24 | 0.58 |
| 2:BJ:49:LEU:HB3 | 2:BJ:50:PRO:HD3 | 1.85 | 0.58 |
| 2:BJ:522:THR:HG22 | 2:BJ:536:TYR:HB3 | 1.86 | 0.58 |
| 2:C:1012:LEU:HD13 | 2:C:1027:GLN:NE2 | 2.18 | 0.58 |
| 2:C:561:TRP:CZ3 | 2:C:566:CYS:HB2 | 2.38 | 0.58 |
| 2:C:781:LEU:HB2 | 2:C:798:ILE:HD11 | 1.86 | 0.58 |
| 2:C:850:ASN:HB3 | 2:GF:581:TYR:OH | 2.03 | 0.58 |
| 4:CC:165:GLU:HB3 | 4:CE:171:LYS:HB2 | 1.85 | 0.58 |
| 5:CG:310:GLU:HB2 | 5:CG:384:THR:HB | 1.84 | 0.58 |
| 5:CF:154:ILE:HB | 5:CH:156:SER:HB2 | 1.85 | 0.58 |
| 7:DC:118:PRO:O | 7:DC:122:THR:N | 2.36 | 0.58 |
| 7:DC:77:THR:HG23 | 7:DC:79:ALA:N | 2.19 | 0.58 |
| 7:DD:47:VAL:HA | 7:DD:57:ILE:HD12 | 1.85 | 0.58 |
| 1:EA:87:SER:OG | 1:EA:230:ILE:O | 2.21 | 0.58 |
| 1:EA:431:GLU:HG2 | 1:EA:435:TRP:CE3 | 2.39 | 0.58 |
| 1:EB:206:TRP:CD1 | 1:EB:222:THR:HB | 2.38 | 0.58 |
| 2:EC:715:LEU:HG | 2:EC:716:ASN:H | 1.67 | 0.58 |
| 2:EC:781:LEU:HB2 | 2:EC:798:ILE:HD11 | 1.86 | 0.58 |
| 2:EC:963:TYR:CD1 | 2:EC:964:PRO:HD2 | 2.39 | 0.58 |
| 4:F:46:ARG:NH2 | 4:F:66:TYR:OH | 2.36 | 0.58 |
| 6:FB:58:ASP:OD1 | 6:FC:164:GLN:NE2 | 2.36 | 0.58 |
| 6:FB:11:ILE:HA | 6:FD:7:LYS:HD3 | 1.85 | 0.58 |
| 12:DJ:137:TYR:OH | 12:GC:157:PRO:HD3 | 2.04 | 0.58 |
| 1:GE:363:PHE:CD1 | 1:GE:636:ASP:HB2 | 2.39 | 0.58 |
| 2:GF:977:ILE:HD12 | 2:GF:981:GLN:HA | 1.85 | 0.58 |
| 4:GI:46:ARG:NH2 | 4:GI:66:TYR:OH | 2.36 | 0.58 |
| 5:HB:146:VAL:HG23 | 5:HC:153:LYS:HB2 | 1.85 | 0.58 |
| 5:HC:5:ILE:HD11 | 5:HC:22:GLY:HA2 | 1.84 | 0.58 |
| 5:HD:328:LEU:HD12 | 5:HD:330:HIS:CD2 | 2.38 | 0.58 |
| 7:HH:101:SER:OG | 7:HH:106:ALA:N | 2.36 | 0.58 |
| 7:HH:20:PRO:CD | 7:HH:29:ILE:HG21 | 2.33 | 0.58 |
| 7:HI:147:LEU:HB2 | 7:HI:148:PRO:HD3 | 1.84 | 0.58 |
| 7:HJ:132:ARG:NH1 | 7:HJ:139:ASN:O | 2.36 | 0.58 |
| 7:HJ:466:SER:HB3 | 7:HJ:468:PHE:HE2 | 1.68 | 0.58 |
| 8:IB:27:TYR:HD2 | 8:IB:28:LEU:HD12 | 1.69 | 0.58 |
| 9:IC:75:ARG:HG3 | 10:ID:123:PRO:HG3 | 1.85 | 0.58 |
| 5:J:132:ASP:OD2 | 5:J:151:ILE:N | 2.36 | 0.58 |
| 5:K:359:GLU:HB3 | 5:K:370:HIS:HB3 | 1.84 | 0.58 |
| 5:K:371:PHE:CZ | 5:K:373:SER:HB3 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:L:73:ASN:HA | 6:N:70:ILE:HG12 | 1.83 | 0.58 |
| 7:O:512:THR:HA | 7:P:442:MET:HA | 1.85 | 0.58 |
| 7:Q:20:PRO:HB3 | 7:Q:29:ILE:HG13 | 1.85 | 0.58 |
| 12:W:104:PHE:HZ | 12:IF:213:ALA:HB3 | 1.68 | 0.58 |
| 1:X:544:ASP:HB2 | 1:X:576:ASP:CG | 2.24 | 0.58 |
| 13:YA:17[E]:ASP:OD1 | 13:YA:19[E]:MET:N | 2.37 | 0.58 |
| 13:YA:169[F]:ASP:HB2 | 13:YA:343[F]:VAL:HB | 1.86 | 0.58 |
| 13:YB:320[A]:THR:HB | 13:YB:324[A]:ALA:HB2 | 1.84 | 0.58 |
| 13:YB:424[F]:VAL:HA | 13:YB:429[F]:ARG:O | 2.04 | 0.58 |
| 13:YB:567[F]:ILE:HG23 | 13:YC:565[F]:TYR:CE2 | 2.38 | 0.58 |
| 13:YB:25[C]:GLY:HA3 | 13:YB:73[C]:VAL:HG12 | 1.85 | 0.58 |
| 13:YC:387[D]:TYR:CZ | 13:YC:388[D]:PRO:HB3 | 2.38 | 0.58 |
| 13:YC:387[A]:TYR:CZ | 13:YC:388[A]:PRO:HB3 | 2.38 | 0.58 |
| 13:YA:555[E]:ALA:O | 13:YC:563[E]:GLY:N | 2.36 | 0.58 |
| 14:YD:46[A]:GLY:HA3 | 14:YD:174[A]:ARG:HH22 | 1.67 | 0.58 |
| 14:YE:46[D]:GLY:HA3 | 14:YE:174[D]:ARG:HH22 | 1.68 | 0.58 |
| 14:YE:84[D]:LYS:NZ | 14:YE:317[D]:ASN:OD1 | 2.36 | 0.58 |
| 11:BF:178:ASN:N | 14:YF:217[E]:SER:O | 2.34 | 0.58 |
| 14:YF:70[B]:ILE:HG21 | 14:YF:109[B]:LEU:HD21 | 1.86 | 0.58 |
| 2:Z:376:PHE:HB3 | 2:Z:405:VAL:HA | 1.86 | 0.58 |
| 2:Z:39:ALA:HB1 | 2:Z:54:TYR:HE1 | 1.68 | 0.58 |
| 5:AC:326:MET:CE | 5:AD:264:ARG:HB3 | 2.34 | 0.58 |
| 5:AD:139:ALA:HB3 | 5:AE:99:PHE:HB3 | 1.85 | 0.58 |
| 8:BB:27:TYR:HD2 | 8:BB:28:LEU:HD12 | 1.69 | 0.58 |
| 1:BH:494:THR:HG21 | 1:BH:603:TYR:HA | 1.86 | 0.58 |
| 2:BJ:338:PHE:HE2 | 2:BJ:342:SER:O | 1.87 | 0.58 |
| 2:BJ:561:TRP:CZ3 | 2:BJ:566:CYS:HB2 | 2.38 | 0.58 |
| 2:BJ:575:PHE:HB2 | 2:BJ:608:VAL:HG22 | 1.85 | 0.58 |
| 2:BJ:578:PHE:CE2 | 2:BJ:582:ALA:HB2 | 2.38 | 0.58 |
| 2:BJ:816:LEU:H | 3:CB:201:ASN:ND2 | 2.02 | 0.58 |
| 3:CB:177:GLU:HG3 | 3:CB:180:ILE:HG22 | 1.86 | 0.58 |
| 3:CB:195:PRO:HD3 | 3:CB:223:TRP:HD1 | 1.65 | 0.58 |
| 4:CD:46:ARG:NH2 | 4:CD:66:TYR:OH | 2.36 | 0.58 |
| 4:CE:46:ARG:NH2 | 4:CE:66:TYR:OH | 2.36 | 0.58 |
| 5:CG:263:ILE:HG22 | 5:CG:381:ILE:HB | 1.86 | 0.58 |
| 5:CG:542:LEU:HD11 | 5:CH:569:TYR:CE2 | 2.39 | 0.58 |
| 7:DB:481:SER:OG | 7:DC:449:GLY:O | 2.15 | 0.58 |
| 7:DD:4:ASN:OD1 | 7:DD:15:TYR:OH | 2.17 | 0.58 |
| 1:EA:145:PHE:CB | 1:EA:169:GLN:HA | 2.32 | 0.58 |
| 1:EA:502:ASN:N | 1:EA:600:ASP:OD2 | 2.37 | 0.58 |
| 1:EB:330:THR:O | 1:EB:333:ARG:HG2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:555:ARG:HG3 | 2:EC:557:VAL:H | 1.68 | 0.58 |
| 2:EC:724:ALA:O | 2:EC:726:PHE:N | 2.36 | 0.58 |
| 5:FA:213:GLY:O | 5:FA:221:GLU:HB2 | 2.04 | 0.58 |
| 7:FE:43:GLY:O | 7:FF:42:ALA:HB3 | 2.04 | 0.58 |
| 7:FF:233:GLN:HE21 | 7:FF:237:ASN:ND2 | 2.01 | 0.58 |
| 7:FE:260:ARG:NH1 | 7:FG:251:ASN:O | 2.37 | 0.58 |
| 2:GF:1012:LEU:HD13 | 2:GF:1027:GLN:NE2 | 2.18 | 0.58 |
| 3:GG:24:PHE:O | 3:GG:27:SER:OG | 2.19 | 0.58 |
| 5:HC:419:ASP:HB3 | 5:HC:436:VAL:HB | 1.86 | 0.58 |
| 5:HD:563:GLY:O | 5:HD:565:ILE:N | 2.34 | 0.58 |
| 7:HI:422:LYS:NZ | 7:HJ:498:SER:O | 2.36 | 0.58 |
| 7:HJ:12:GLU:HB3 | 7:HJ:15:TYR:HB3 | 1.84 | 0.58 |
| 10:ID:288:SER:OG | 10:ID:289:ASN:N | 2.36 | 0.58 |
| 10:ID:37:GLN:N | 10:ID:37:GLN:OE1 | 2.36 | 0.58 |
| 5:J:253:GLN:HE22 | 5:K:249:ASP:HB3 | 1.69 | 0.58 |
| 5:J:419:ASP:HB3 | 5:J:436:VAL:HB | 1.86 | 0.58 |
| 5:J:72:THR:HG22 | 5:J:77:VAL:HG22 | 1.85 | 0.58 |
| 5:K:92:VAL:HG12 | 5:K:136:VAL:HG12 | 1.85 | 0.58 |
| 7:O:445:HIS:CE1 | 7:P:445:HIS:NE2 | 2.71 | 0.58 |
| 7:O:359:TRP:NE1 | 7:P:340:THR:O | 2.28 | 0.58 |
| 7:Q:466:SER:HB3 | 7:Q:468:PHE:HE2 | 1.68 | 0.58 |
| 7:Q:525:VAL:HG23 | 7:Q:526:LYS:HG2 | 1.84 | 0.58 |
| 8:S:53:PHE:CD2 | 8:S:54:MET:HG2 | 2.39 | 0.58 |
| 9:T:98:VAL:HB | 9:T:103:THR:HB | 1.86 | 0.58 |
| 1:X:209:TRP:HD1 | 1:X:225:TYR:HE1 | 1.51 | 0.58 |
| 1:X:424:TYR:HA | 1:X:476:ILE:HG12 | 1.86 | 0.58 |
| 13:YB:17[E]:ASP:OD1 | 13:YB:19[E]:MET:N | 2.36 | 0.58 |
| 13:YB:320[B]:THR:HB | 13:YB:324[B]:ALA:HB2 | 1.84 | 0.58 |
| 13:YB:169[E]:ASP:HB2 | 13:YB:343[E]:VAL:HB | 1.86 | 0.58 |
| 13:YB:387[A]:TYR:CZ | 13:YB:388[A]:PRO:HB3 | 2.38 | 0.58 |
| 13:YB:416[E]:HIS:CD2 | 13:YB:418[E]:THR:H | 2.21 | 0.58 |
| 13:YC:17[A]:ASP:OD1 | 13:YC:19[A]:MET:N | 2.37 | 0.58 |
| 13:YC:424[D]:VAL:HA | 13:YC:429[D]:ARG:O | 2.04 | 0.58 |
| 13:YC:424[E]:VAL:HA | 13:YC:429[E]:ARG:O | 2.04 | 0.58 |
| 13:YA:83[B]:TYR:CZ | 13:YC:95[B]:ILE:HD11 | 2.39 | 0.58 |
| 14:YD:232[B]:TYR:OH | 14:YD:312[B]:THR:O | 2.21 | 0.58 |
| 11:IE:190:LYS:HE3 | 14:YE:24[E]:SER:O | 2.04 | 0.58 |
| 14:YF:46[C]:GLY:HA3 | 14:YF:174[C]:ARG:HH22 | 1.67 | 0.58 |
| 14:YF:46[D]:GLY:HA3 | 14:YF:174[D]:ARG:HH22 | 1.68 | 0.58 |
| 2:Z:435:SER:HB3 | 2:Z:512:PRO:HA | 1.86 | 0.58 |
| 1:A:77:GLU:OE2 | 1:A:88:SER:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:212:PRO:HG3 | 7:AJ:199:VAL:HG12 | 1.85 | 0.58 |
| 1:B:208:ASN:HB3 | 1:B:224:TYR:CE1 | 2.38 | 0.58 |
| 7:BA:466:SER:HB3 | 7:BA:468:PHE:HE2 | 1.69 | 0.58 |
| 8:BB:120:ALA:HB3 | 8:DF:99:ILE:O | 2.04 | 0.58 |
| 11:BF:110:VAL:HG22 | 11:BF:111:TYR:HD2 | 1.68 | 0.58 |
| 1:BI:455:PHE:CD2 | 1:BI:456:ASN:HB2 | 2.38 | 0.58 |
| 2:BJ:675:LEU:O | 2:BJ:681:THR:HB | 2.04 | 0.58 |
| 2:BJ:775:ASP:O | 2:BJ:776:SER:OG | 2.20 | 0.58 |
| 2:BJ:768:TYR:OH | 2:BJ:814:HIS:O | 2.17 | 0.58 |
| 2:BJ:848:LEU:O | 2:BJ:850:ASN:N | 2.37 | 0.58 |
| 3:CA:95:TRP:CH2 | 3:CA:169:PRO:HD3 | 2.38 | 0.58 |
| 4:CC:218:GLU:OE1 | 4:CD:201:LYS:NZ | 2.31 | 0.58 |
| 5:CH:469:PRO:HA | 5:CH:472:TYR:CE2 | 2.39 | 0.58 |
| 7:DB:512:THR:HA | 7:DC:442:MET:HA | 1.85 | 0.58 |
| 7:DC:360:ARG:NH1 | 7:DC:525:VAL:HG21 | 2.18 | 0.58 |
| 9:DG:53:PHE:HA | 9:DG:84:TYR:CE2 | 2.39 | 0.58 |
| 1:EA:544:ASP:HB2 | 1:EA:576:ASP:CG | 2.24 | 0.58 |
| 1:EA:558:PHE:O | 1:EA:586:ARG:HB2 | 2.04 | 0.58 |
| 2:EC:1013:LYS:HE3 | 2:EC:1022:PRO:HG3 | 1.85 | 0.58 |
| 2:EC:316:ASP:O | 2:EC:331:THR:N | 2.34 | 0.58 |
| 5:EI:139:ALA:HB3 | 5:EJ:99:PHE:HB3 | 1.86 | 0.58 |
| 7:FG:47:VAL:HA | 7:FG:57:ILE:HD12 | 1.85 | 0.58 |
| 12:GC:204:HIS:HB3 | 12:GC:210:PRO:HA | 1.86 | 0.58 |
| 1:GD:112:LEU:HB2 | 1:GD:300:ILE:HG22 | 1.86 | 0.58 |
| 1:GD:424:TYR:HA | 1:GD:476:ILE:HG12 | 1.86 | 0.58 |
| 1:GE:208:ASN:HB3 | 1:GE:224:TYR:CE1 | 2.38 | 0.58 |
| 2:GF:675:LEU:O | 2:GF:681:THR:HB | 2.04 | 0.58 |
| 3:GH:177:GLU:HG3 | 3:GH:180:ILE:HG22 | 1.86 | 0.58 |
| 4:H:46:ARG:NH2 | 4:H:66:TYR:OH | 2.36 | 0.58 |
| 5:HB:426:ASP:O | 5:HB:479:LYS:NZ | 2.36 | 0.58 |
| 5:HD:102:TRP:HE3 | 5:HD:131:SER:HB2 | 1.67 | 0.58 |
| 5:HD:490:TRP:NE1 | 5:HD:515:THR:O | 2.37 | 0.58 |
| 5:HC:356:TYR:HE1 | 6:HE:4:LEU:HD13 | 1.68 | 0.58 |
| 7:HH:445:HIS:CE1 | 7:HI:445:HIS:NE2 | 2.72 | 0.58 |
| 7:HJ:142:ILE:HG21 | 7:HJ:157:THR:O | 2.04 | 0.58 |
| 7:HJ:296:ILE:HG22 | 7:HJ:298:GLY:H | 1.67 | 0.58 |
| 5:I:187:ASN:HB2 | 5:I:254:TRP:CZ2 | 2.39 | 0.58 |
| 5:I:146:VAL:HG23 | 5:J:153:LYS:HB2 | 1.85 | 0.58 |
| 5:J:164:ARG:HG3 | 5:J:245:GLU:HG2 | 1.86 | 0.58 |
| 5:J:206:PHE:CZ | 5:J:221:GLU:HG2 | 2.38 | 0.58 |
| 5:K:213:GLY:O | 5:K:221:GLU:HB2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:469:PRO:HA | 5:K:472:TYR:CE2 | 2.39 | 0.58 |
| 8:R:53:PHE:CD2 | 8:R:54:MET:HG2 | 2.39 | 0.58 |
| 1:B:23:GLY:N | 11:V:26:THR:OG1 | 2.22 | 0.58 |
| 1:X:145:PHE:HZ | 1:X:286:PHE:HE1 | 1.52 | 0.58 |
| 1:X:484:MET:HE1 | 1:X:501:TYR:HB3 | 1.86 | 0.58 |
| 1:Y:206:TRP:CD1 | 1:Y:222:THR:HB | 2.38 | 0.58 |
| 13:YA:17[D]:ASP:OD1 | 13:YA:19[D]:MET:N | 2.37 | 0.58 |
| 13:YA:424[A]:VAL:HA | 13:YA:429[A]:ARG:O | 2.04 | 0.58 |
| 13:YA:424[C]:VAL:HA | 13:YA:429[C]:ARG:O | 2.04 | 0.58 |
| 13:YA:555[C]:ALA:O | 13:YC:563[C]:GLY:N | 2.36 | 0.58 |
| 13:YB:416[D]:HIS:CD2 | 13:YB:418[D]:THR:H | 2.21 | 0.58 |
| 13:YB:424[A]:VAL:HA | 13:YB:429[A]:ARG:O | 2.04 | 0.58 |
| 13:YB:424[E]:VAL:HA | 13:YB:429[E]:ARG:O | 2.04 | 0.58 |
| 13:YB:437[E]:ASN:HB3 | 13:YB:439[E]:TYR:HE1 | 1.66 | 0.58 |
| 13:YC:320[F]:THR:HB | 13:YC:324[F]:ALA:HB2 | 1.85 | 0.58 |
| 13:YC:65[F]:ALA:N | 13:YC:69[F]:ILE:O | 2.36 | 0.58 |
| 13:YC:57[A]:VAL:CG1 | 13:YC:76[A]:PRO:HD3 | 2.34 | 0.58 |
| 14:YE:70[B]:ILE:HG21 | 14:YE:109[B]:LEU:HD21 | 1.86 | 0.58 |
| 13:YC:90[E]:TRP:NE1 | 14:YF:175[E]:GLU:OE1 | 2.35 | 0.58 |
| 2:Z:529:SER:O | 2:Z:531:ARG:HG3 | 2.04 | 0.58 |
| 2:Z:675:LEU:O | 2:Z:681:THR:HB | 2.04 | 0.58 |
| 2:Z:781:LEU:HB2 | 2:Z:798:ILE:HD11 | 1.86 | 0.58 |
| 4:AA:239:ARG:HD2 | 4:AA:249:ILE:HD12 | 1.85 | 0.58 |
| 5:AD:193:VAL:HG13 | 5:AD:199:GLU:HB3 | 1.86 | 0.58 |
| 5:AD:72:THR:HG22 | 5:AD:77:VAL:HG22 | 1.85 | 0.58 |
| 5:AE:89:TYR:O | 5:AE:91:LYS:HG2 | 2.04 | 0.58 |
| 6:AF:13:ARG:HB2 | 6:AH:10:VAL:HA | 1.86 | 0.58 |
| 7:AI:514:PRO:HB3 | 7:AJ:512:THR:O | 2.04 | 0.58 |
| 7:AJ:77:THR:HG23 | 7:AJ:79:ALA:N | 2.19 | 0.58 |
| 1:B:83:ALA:O | 1:B:326:ARG:NH2 | 2.36 | 0.58 |
| 7:BA:145:SER:O | 7:BA:164:LYS:NZ | 2.25 | 0.58 |
| 7:BA:20:PRO:HB3 | 7:BA:29:ILE:HG13 | 1.84 | 0.58 |
| 12:BG:137:TYR:OH | 12:DJ:157:PRO:HD3 | 2.04 | 0.58 |
| 12:BG:20:ASN:OD1 | 12:DJ:233:ASP:HA | 2.04 | 0.58 |
| 2:BJ:724:ALA:O | 2:BJ:726:PHE:N | 2.36 | 0.58 |
| 2:C:1013:LYS:HE3 | 2:C:1022:PRO:HG3 | 1.85 | 0.58 |
| 2:C:929:TYR:CZ | 2:C:963:TYR:HD1 | 2.22 | 0.58 |
| 3:CA:46:PRO:HG3 | 3:CA:270:ARG:HH22 | 1.68 | 0.58 |
| 4:CE:131:LYS:N | 4:CE:160:TRP:O | 2.29 | 0.58 |
| 4:CE:40:ASN:HB3 | 4:CE:45:GLN:HG2 | 1.85 | 0.58 |
| 5:CF:44:TYR:HD2 | 5:CF:48:ALA:HB2 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:206:PHE:CZ | 5:CG:221:GLU:HG2 | 2.38 | 0.58 |
| 7:DB:112:ASN:HA | 7:DD:117:THR:OG1 | 2.03 | 0.58 |
| 7:DB:340:THR:HG22 | 7:DB:341:ILE:HG12 | 1.85 | 0.58 |
| 8:DE:68:ASP:OD1 | 8:DE:69:TRP:N | 2.36 | 0.58 |
| 12:DJ:204:HIS:HB3 | 12:DJ:210:PRO:HA | 1.86 | 0.58 |
| 1:EA:484:MET:HE1 | 1:EA:501:TYR:HB3 | 1.86 | 0.58 |
| 4:F:202:LEU:HB3 | 4:F:278:VAL:HG22 | 1.86 | 0.58 |
| 5:FA:313:PHE:CE2 | 5:FA:320:LEU:HD21 | 2.39 | 0.58 |
| 8:FH:38:ALA:HB3 | 8:FH:72:THR:HG22 | 1.85 | 0.58 |
| 12:GC:161:SER:HB3 | 12:GC:240:ASP:HB3 | 1.85 | 0.58 |
| 2:GF:929:TYR:CZ | 2:GF:963:TYR:HD1 | 2.22 | 0.58 |
| 5:HB:187:ASN:HB2 | 5:HB:254:TRP:CZ2 | 2.39 | 0.58 |
| 5:HC:44:TYR:CD2 | 5:HC:48:ALA:HB2 | 2.37 | 0.58 |
| 7:HI:77:THR:HG23 | 7:HI:79:ALA:N | 2.19 | 0.58 |
| 7:HJ:47:VAL:HA | 7:HJ:57:ILE:HD12 | 1.85 | 0.58 |
| 5:I:154:ILE:HB | 5:K:156:SER:HB2 | 1.85 | 0.58 |
| 8:IA:27:TYR:HD2 | 8:IA:28:LEU:HD12 | 1.69 | 0.58 |
| 5:J:176:ASP:HA | 5:J:231:ARG:HA | 1.85 | 0.58 |
| 5:J:263:ILE:HG22 | 5:J:381:ILE:HB | 1.86 | 0.58 |
| 5:J:310:GLU:HB2 | 5:J:384:THR:HB | 1.84 | 0.58 |
| 5:K:398:GLU:OE1 | 5:K:398:GLU:N | 2.37 | 0.58 |
| 7:P:386:ASN:HB2 | 7:P:387:PRO:HD2 | 1.85 | 0.58 |
| 7:Q:132:ARG:NH1 | 7:Q:139:ASN:O | 2.36 | 0.58 |
| 8:R:34:PHE:HD2 | 8:IA:9:ALA:HB2 | 1.69 | 0.58 |
| 1:X:53:LEU:HD12 | 1:X:53:LEU:O | 2.03 | 0.58 |
| 1:X:77:GLU:OE2 | 1:X:88:SER:HB2 | 2.03 | 0.58 |
| 13:YA:437[A]:ASN:HB3 | 13:YA:439[A]:TYR:HE1 | 1.67 | 0.58 |
| 13:YA:534[F]:LEU:HB2 | 13:YC:538[F]:VAL:HG11 | 1.85 | 0.58 |
| 13:YB:416[C]:HIS:HD2 | 13:YB:418[C]:THR:H | 1.51 | 0.58 |
| 13:YA:554[C]:MET:HE2 | 13:YB:550[C]:TRP:CD1 | 2.39 | 0.58 |
| 13:YB:57[A]:VAL:CG1 | 13:YB:76[A]:PRO:HD3 | 2.34 | 0.58 |
| 13:YC:424[C]:VAL:HA | 13:YC:429[C]:ARG:O | 2.04 | 0.58 |
| 13:YB:434[A]:THR:HG21 | 13:YC:430[A]:ARG:HB3 | 1.85 | 0.58 |
| 2:Z:241:SER:HB2 | 2:Z:313:CYS:SG | 2.44 | 0.58 |
| 2:Z:575:PHE:HB2 | 2:Z:608:VAL:HG22 | 1.85 | 0.58 |
| 2:Z:977:ILE:HD12 | 2:Z:981:GLN:HA | 1.85 | 0.58 |
| 4:AA:36:ASN:OD1 | 4:AB:7:LYS:NZ | 2.23 | 0.57 |
| 4:AA:40:ASN:HB3 | 4:AA:45:GLN:HG2 | 1.85 | 0.57 |
| 5:AC:183:GLY:HA2 | 5:AC:307:ASN:HD22 | 1.68 | 0.57 |
| 5:AD:213:GLY:O | 5:AD:214:SER:OG | 2.22 | 0.57 |
| 7:AI:375:TYR:HE2 | 7:AI:390:PRO:HB2 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:360:ARG:NH1 | 7:AJ:525:VAL:HG21 | 2.18 | 0.57 |
| 7:AI:422:LYS:HB3 | 7:AJ:504:ARG:HA | 1.86 | 0.57 |
| 1:BI:209:TRP:HE3 | 1:BI:212:LYS:HB2 | 1.69 | 0.57 |
| 2:BJ:977:ILE:HD12 | 2:BJ:981:GLN:HA | 1.85 | 0.57 |
| 2:C:189:ARG:HG2 | 2:C:204:ARG:HH12 | 1.69 | 0.57 |
| 2:C:241:SER:HB2 | 2:C:313:CYS:SG | 2.44 | 0.57 |
| 2:C:77:THR:HG22 | 2:C:101:GLU:HB3 | 1.87 | 0.57 |
| 5:CF:213:GLY:O | 5:CF:214:SER:OG | 2.22 | 0.57 |
| 5:CF:569:TYR:CD1 | 5:CG:544:VAL:HA | 2.39 | 0.57 |
| 5:CG:334:ALA:O | 5:CG:337:ASP:N | 2.35 | 0.57 |
| 5:CG:62:ALA:HB1 | 5:CG:82:PRO:HG3 | 1.85 | 0.57 |
| 5:CH:328:LEU:HD12 | 5:CH:330:HIS:CD2 | 2.38 | 0.57 |
| 5:CH:490:TRP:NE1 | 5:CH:515:THR:O | 2.36 | 0.57 |
| 6:CI:107:VAL:O | 6:CI:114:VAL:N | 2.37 | 0.57 |
| 7:DB:12:GLU:HB3 | 7:DB:15:TYR:HB3 | 1.86 | 0.57 |
| 2:EC:64:ASN:OD1 | 2:EC:65:ASN:N | 2.33 | 0.57 |
| 2:EC:773:GLN:N | 2:EC:837:GLU:O | 2.33 | 0.57 |
| 4:EG:239:ARG:HD2 | 4:EG:249:ILE:HD12 | 1.85 | 0.57 |
| 4:EG:46:ARG:NH2 | 4:EG:66:TYR:OH | 2.36 | 0.57 |
| 4:EF:7:LYS:HB2 | 4:EH:39:TYR:CD1 | 2.39 | 0.57 |
| 5:EJ:4:ASN:OD1 | 5:EJ:5:ILE:N | 2.36 | 0.57 |
| 5:FA:291:ILE:HG22 | 5:FA:292:PRO:O | 2.04 | 0.57 |
| 5:FA:371:PHE:CZ | 5:FA:373:SER:HB3 | 2.38 | 0.57 |
| 8:FH:27:TYR:HD2 | 8:FH:28:LEU:HD12 | 1.69 | 0.57 |
| 4:G:46:ARG:NH2 | 4:G:66:TYR:OH | 2.36 | 0.57 |
| 10:GA:37:GLN:OE1 | 10:GA:37:GLN:N | 2.36 | 0.57 |
| 12:GC:177:TRP:CZ3 | 12:GC:220:SER:HB3 | 2.38 | 0.57 |
| 12:GC:22:PHE:HA | 12:GC:203:LEU:HA | 1.86 | 0.57 |
| 1:GD:77:GLU:OE2 | 1:GD:88:SER:HB2 | 2.03 | 0.57 |
| 1:GE:452:VAL:O | 1:GE:457:SER:OG | 2.22 | 0.57 |
| 2:GF:241:SER:HB2 | 2:GF:313:CYS:SG | 2.44 | 0.57 |
| 2:GF:435:SER:HB3 | 2:GF:512:PRO:HA | 1.86 | 0.57 |
| 2:GF:935:LYS:HZ2 | 2:GF:936:LEU:HD13 | 1.68 | 0.57 |
| 2:GF:929:TYR:CD2 | 2:GF:961:VAL:HB | 2.39 | 0.57 |
| 4:GJ:46:ARG:NH2 | 4:GJ:66:TYR:OH | 2.37 | 0.57 |
| 5:HB:285:LEU:HD21 | 5:HB:375:PHE:H | 1.68 | 0.57 |
| 5:HC:206:PHE:CZ | 5:HC:221:GLU:HG2 | 2.38 | 0.57 |
| 5:HD:291:ILE:HG22 | 5:HD:292:PRO:O | 2.04 | 0.57 |
| 6:HG:107:VAL:O | 6:HG:114:VAL:N | 2.37 | 0.57 |
| 8:S:99:ILE:O | 8:IA:120:ALA:HB3 | 2.04 | 0.57 |
| 8:IA:53:PHE:CD2 | 8:IA:54:MET:HG2 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:ID:214:ARG:NH1 | 12:IF:246:ARG:HH12 | 1.99 | 0.57 |
| 5:J:216:GLY:H | 5:J:231:ARG:HB2 | 1.68 | 0.57 |
| 5:I:520:GLY:O | 5:K:591:PRO:HA | 2.04 | 0.57 |
| 7:Q:453:GLU:OE2 | 7:Q:471:THR:N | 2.29 | 0.57 |
| 12:W:204:HIS:HB3 | 12:W:210:PRO:HA | 1.86 | 0.57 |
| 1:X:582:ASN:OD1 | 1:X:585:GLY:N | 2.27 | 0.57 |
| 1:X:494:THR:HG21 | 1:X:603:TYR:HA | 1.86 | 0.57 |
| 1:Y:174:ARG:NH2 | 1:Y:269:VAL:HG21 | 2.18 | 0.57 |
| 1:Y:440:ILE:HD11 | 1:Y:653:ILE:HG12 | 1.85 | 0.57 |
| 13:YA:17[A]:ASP:OD1 | 13:YA:19[A]:MET:N | 2.37 | 0.57 |
| 13:YA:399[C]:HIS:CD2 | 13:YB:403[C]:PHE:HB3 | 2.39 | 0.57 |
| 13:YA:434[C]:THR:O | 13:YC:442[C]:THR:HA | 2.03 | 0.57 |
| 13:YA:558[A]:SER:HB3 | 13:YB:551[A]:THR:HG22 | 1.84 | 0.57 |
| 13:YB:47[B]:ILE:HG23 | 14:YE:123[B]:PRO:CG | 2.31 | 0.57 |
| 13:YB:25[D]:GLY:HA3 | 13:YB:73[D]:VAL:HG12 | 1.86 | 0.57 |
| 13:YB:82[A]:VAL:HG22 | 13:YB:98[A]:GLY:O | 2.04 | 0.57 |
| 13:YC:320[E]:THR:HB | 13:YC:324[E]:ALA:HB2 | 1.84 | 0.57 |
| 13:YB:291[D]:LYS:HZ3 | 13:YC:362[D]:ASP:N | 2.02 | 0.57 |
| 13:YA:59[C]:GLN:CA | 13:YC:61[C]:ILE:HG21 | 2.33 | 0.57 |
| 13:YA:83[A]:TYR:CZ | 13:YC:95[A]:ILE:HD11 | 2.39 | 0.57 |
| 14:YF:70[A]:ILE:HG21 | 14:YF:109[A]:LEU:HD21 | 1.86 | 0.57 |
| 2:Z:189:ARG:HG2 | 2:Z:204:ARG:HH12 | 1.69 | 0.57 |
| 5:AC:162:VAL:O | 5:AD:253:GLN:HA | 2.04 | 0.57 |
| 5:AD:136:VAL:O | 5:AD:143:TRP:HA | 2.04 | 0.57 |
| 5:AD:263:ILE:HG22 | 5:AD:381:ILE:HB | 1.86 | 0.57 |
| 5:AE:469:PRO:HA | 5:AE:472:TYR:CE2 | 2.39 | 0.57 |
| 5:AE:563:GLY:O | 5:AE:565:ILE:N | 2.34 | 0.57 |
| 7:AI:340:THR:HG22 | 7:AI:341:ILE:HG12 | 1.84 | 0.57 |
| 7:AJ:118:PRO:O | 7:AJ:122:THR:N | 2.37 | 0.57 |
| 1:B:452:VAL:O | 1:B:457:SER:OG | 2.22 | 0.57 |
| 8:BC:27:TYR:HD2 | 8:BC:28:LEU:HD12 | 1.69 | 0.57 |
| 8:BC:89:GLN:HB3 | 8:BC:134:PRO:HG2 | 1.85 | 0.57 |
| 1:BH:112:LEU:HB2 | 1:BH:300:ILE:HG22 | 1.86 | 0.57 |
| 1:BH:424:TYR:HA | 1:BH:476:ILE:HG12 | 1.86 | 0.57 |
| 1:BH:502:ASN:N | 1:BH:600:ASP:OD2 | 2.37 | 0.57 |
| 2:BJ:168:ILE:HG12 | 2:BJ:578:PHE:HZ | 1.69 | 0.57 |
| 2:BJ:581:TYR:OH | 2:EC:850:ASN:HB3 | 2.04 | 0.57 |
| 2:BJ:872:SER:O | 2:BJ:873:SER:OG | 2.16 | 0.57 |
| 2:C:575:PHE:HB2 | 2:C:608:VAL:HG22 | 1.85 | 0.57 |
| 3:CA:48:SER:OG | 3:CA:49:SER:N | 2.37 | 0.57 |
| 5:CF:187:ASN:HB2 | 5:CF:254:TRP:CZ2 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:146:VAL:HG23 | 5:CG:153:LYS:HB2 | 1.85 | 0.57 |
| 5:CG:176:ASP:HA | 5:CG:231:ARG:HA | 1.85 | 0.57 |
| 7:DB:445:HIS:CE1 | 7:DC:445:HIS:NE2 | 2.71 | 0.57 |
| 12:DJ:19:ASN:OD1 | 12:GC:228:LEU:HA | 2.05 | 0.57 |
| 1:EB:102:SER:N | 1:EB:194:ARG:HH12 | 2.00 | 0.57 |
| 2:EC:522:THR:HG22 | 2:EC:536:TYR:HB3 | 1.86 | 0.57 |
| 2:EC:848:LEU:O | 2:EC:850:ASN:N | 2.37 | 0.57 |
| 1:EB:496:GLU:HG3 | 2:EC:856:ASN:O | 2.04 | 0.57 |
| 4:EF:275:ALA:O | 4:EG:282:GLN:NE2 | 2.37 | 0.57 |
| 5:EJ:240:ASP:OD1 | 7:FG:4:ASN:ND2 | 2.37 | 0.57 |
| 5:EI:407:TYR:HD2 | 5:EJ:407:TYR:CD2 | 2.23 | 0.57 |
| 6:FB:107:VAL:O | 6:FB:114:VAL:N | 2.37 | 0.57 |
| 6:FC:57:ASN:HB2 | 6:FD:164:GLN:NE2 | 2.18 | 0.57 |
| 7:FF:77:THR:HG23 | 7:FF:79:ALA:N | 2.19 | 0.57 |
| 8:FI:38:ALA:HB3 | 8:FI:72:THR:HG22 | 1.85 | 0.57 |
| 4:F:69:LYS:NZ | 4:G:103:LEU:O | 2.30 | 0.57 |
| 1:GD:558:PHE:O | 1:GD:586:ARG:HB2 | 2.04 | 0.57 |
| 2:GF:1013:LYS:HE3 | 2:GF:1022:PRO:HG3 | 1.85 | 0.57 |
| 3:GG:48:SER:OG | 3:GG:49:SER:N | 2.37 | 0.57 |
| 5:HC:150:GLN:HB2 | 5:HC:152:ASP:HB3 | 1.84 | 0.57 |
| 5:HC:600:ARG:NE | 5:HC:602:ALA:O | 2.32 | 0.57 |
| 5:HC:49:TRP:HZ3 | 5:HC:96:ARG:HD2 | 1.70 | 0.57 |
| 6:HE:15:ALA:HB2 | 6:HG:52:ILE:HD11 | 1.86 | 0.57 |
| 7:HH:12:GLU:HB3 | 7:HH:15:TYR:HB3 | 1.86 | 0.57 |
| 7:HH:340:THR:HG22 | 7:HH:341:ILE:HG12 | 1.85 | 0.57 |
| 7:HH:375:TYR:HE2 | 7:HH:390:PRO:HB2 | 1.69 | 0.57 |
| 8:IB:53:PHE:CD2 | 8:IB:54:MET:HG2 | 2.39 | 0.57 |
| 8:IB:89:GLN:HB3 | 8:IB:134:PRO:HG2 | 1.85 | 0.57 |
| 9:IC:53:PHE:HA | 9:IC:84:TYR:CE2 | 2.39 | 0.57 |
| 12:IF:22:PHE:HA | 12:IF:203:LEU:HA | 1.86 | 0.57 |
| 5:J:213:GLY:O | 5:J:214:SER:OG | 2.22 | 0.57 |
| 5:J:590:GLN:HE21 | 5:K:486:VAL:HG11 | 1.69 | 0.57 |
| 5:K:328:LEU:HD12 | 5:K:330:HIS:CD2 | 2.38 | 0.57 |
| 7:P:233:GLN:HE21 | 7:P:237:ASN:ND2 | 2.01 | 0.57 |
| 7:O:347:MET:HE3 | 7:P:347:MET:HB3 | 1.85 | 0.57 |
| 8:R:27:TYR:HD2 | 8:R:28:LEU:HD12 | 1.69 | 0.57 |
| 9:T:53:PHE:HA | 9:T:84:TYR:CE2 | 2.39 | 0.57 |
| 10:U:341:THR:HG21 | 12:IF:149:ARG:HB2 | 1.84 | 0.57 |
| 11:V:40:LEU:HD21 | 11:V:45:LEU:HD11 | 1.85 | 0.57 |
| 1:X:399:TYR:O | 1:X:400:ASN:HB2 | 2.04 | 0.57 |
| 1:Y:102:SER:H | 1:Y:194:ARG:NH1 | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:50[F]:GLU:N | 13:YA:50[F]:GLU:OE2 | 2.33 | 0.57 |
| 13:YA:575[F]:GLY:N | 13:YB:567[F]:ILE:O | 2.37 | 0.57 |
| 13:YA:88[E]:ASP:OD1 | 13:YA:88[E]:ASP:N | 2.37 | 0.57 |
| 13:YA:575[B]:GLY:N | 13:YB:567[B]:ILE:O | 2.37 | 0.57 |
| 13:YC:169[E]:ASP:HB2 | 13:YC:343[E]:VAL:HB | 1.86 | 0.57 |
| 13:YC:320[D]:THR:HB | 13:YC:324[D]:ALA:HB2 | 1.84 | 0.57 |
| 13:YC:169[B]:ASP:HB2 | 13:YC:343[B]:VAL:HB | 1.86 | 0.57 |
| 13:YC:424[B]:VAL:HA | 13:YC:429[B]:ARG:O | 2.04 | 0.57 |
| 13:YA:555[D]:ALA:O | 13:YC:563[D]:GLY:N | 2.36 | 0.57 |
| 13:YC:88[A]:ASP:OD1 | 13:YC:88[A]:ASP:N | 2.38 | 0.57 |
| 14:YF:349[B]:ASN:OD1 | 14:YF:350[B]:ASN:N | 2.38 | 0.57 |
| 2:Z:340:PRO:HA | 2:Z:345:TYR:HE1 | 1.67 | 0.57 |
| 2:Z:929:TYR:CD2 | 2:Z:961:VAL:HB | 2.39 | 0.57 |
| 4:AB:239:ARG:HD2 | 4:AB:249:ILE:HD12 | 1.85 | 0.57 |
| 5:AC:469:PRO:HA | 5:AC:472:TYR:CE2 | 2.39 | 0.57 |
| 5:AC:535:THR:O | 5:AE:576:THR:N | 2.32 | 0.57 |
| 5:AD:131:SER:HA | 5:AD:150:GLN:HA | 1.85 | 0.57 |
| 5:AD:590:GLN:HE21 | 5:AE:486:VAL:HG11 | 1.69 | 0.57 |
| 7:AJ:44:VAL:HG21 | 7:BA:25:PHE:HB3 | 1.86 | 0.57 |
| 7:AJ:40:SER:O | 7:BA:24:ASN:ND2 | 2.37 | 0.57 |
| 11:BF:40:LEU:HD21 | 11:BF:45:LEU:HD11 | 1.85 | 0.57 |
| 1:BI:208:ASN:HB3 | 1:BI:224:TYR:CE1 | 2.38 | 0.57 |
| 2:BJ:935:LYS:HZ3 | 2:BJ:936:LEU:HD13 | 1.68 | 0.57 |
| 2:C:154:SER:OG | 2:C:156:SER:OG | 2.13 | 0.57 |
| 4:CC:282:GLN:NE2 | 4:CE:275:ALA:O | 2.37 | 0.57 |
| 5:CF:419:ASP:OD1 | 5:CF:420:VAL:N | 2.37 | 0.57 |
| 5:CG:131:SER:HA | 5:CG:150:GLN:HA | 1.85 | 0.57 |
| 6:CI:10:VAL:HA | 6:CJ:13:ARG:HD2 | 1.85 | 0.57 |
| 7:DB:78:PRO:HB3 | 7:DC:66:VAL:HA | 1.86 | 0.57 |
| 8:DE:27:TYR:HD2 | 8:DE:28:LEU:HD12 | 1.69 | 0.57 |
| 8:DF:27:TYR:HD2 | 8:DF:28:LEU:HD12 | 1.69 | 0.57 |
| 1:EA:424:TYR:HA | 1:EA:476:ILE:HG12 | 1.86 | 0.57 |
| 1:EB:174:ARG:NH2 | 1:EB:269:VAL:HG21 | 2.18 | 0.57 |
| 2:EC:467:LEU:HD11 | 3:GG:56:PHE:H | 1.68 | 0.57 |
| 2:EC:561:TRP:CZ3 | 2:EC:566:CYS:HB2 | 2.38 | 0.57 |
| 3:EE:195:PRO:HD3 | 3:EE:223:TRP:HD1 | 1.65 | 0.57 |
| 4:EH:40:ASN:HB3 | 4:EH:45:GLN:HG2 | 1.85 | 0.57 |
| 5:EI:472:TYR:HB3 | 5:EJ:418:GLY:C | 2.25 | 0.57 |
| 5:EJ:590:GLN:HE21 | 5:FA:486:VAL:HG11 | 1.68 | 0.57 |
| 7:FE:339:ARG:CZ | 7:FG:358:ALA:HB2 | 2.34 | 0.57 |
| 7:FG:142:ILE:HG21 | 7:FG:157:THR:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FI:27:TYR:HD2 | 8:FI:28:LEU:HD12 | 1.69 | 0.57 |
| 10:GA:288:SER:OG | 10:GA:289:ASN:N | 2.36 | 0.57 |
| 1:GD:209:TRP:HD1 | 1:GD:225:TYR:HE1 | 1.51 | 0.57 |
| 1:GD:619:GLN:OE1 | 1:GD:619:GLN:N | 2.36 | 0.57 |
| 1:GE:209:TRP:HE3 | 1:GE:212:LYS:HB2 | 1.69 | 0.57 |
| 2:GF:246:TYR:HE1 | 2:GF:255:TYR:HD1 | 1.51 | 0.57 |
| 1:GD:60:LEU:HD22 | 2:GF:671:TYR:CD1 | 2.40 | 0.57 |
| 1:GE:496:GLU:HG3 | 2:GF:856:ASN:O | 2.04 | 0.57 |
| 3:GG:46:PRO:HG3 | 3:GG:270:ARG:HH22 | 1.68 | 0.57 |
| 3:GH:170:PRO:HB3 | 3:GH:188:TRP:CG | 2.40 | 0.57 |
| 4:GJ:40:ASN:HB3 | 4:GJ:45:GLN:HG2 | 1.85 | 0.57 |
| 4:H:202:LEU:HB3 | 4:H:278:VAL:HG22 | 1.87 | 0.57 |
| 5:HB:213:GLY:O | 5:HB:214:SER:OG | 2.22 | 0.57 |
| 5:HB:594:THR:OG1 | 5:HC:517:GLY:N | 2.37 | 0.57 |
| 5:HC:136:VAL:O | 5:HC:143:TRP:HA | 2.04 | 0.57 |
| 6:HG:192:THR:HB | 6:HG:219:ALA:HB3 | 1.87 | 0.57 |
| 7:HH:513:ARG:O | 7:HI:441:GLN:N | 2.30 | 0.57 |
| 5:I:213:GLY:HA2 | 5:I:221:GLU:HB2 | 1.87 | 0.57 |
| 5:I:419:ASP:OD1 | 5:I:420:VAL:N | 2.37 | 0.57 |
| 5:I:569:TYR:CD1 | 5:J:544:VAL:HA | 2.39 | 0.57 |
| 5:I:30:PHE:HE1 | 5:K:30:PHE:CE1 | 2.22 | 0.57 |
| 5:I:517:GLY:N | 5:K:594:THR:OG1 | 2.37 | 0.57 |
| 6:L:15:ALA:HB2 | 6:N:52:ILE:HD11 | 1.85 | 0.57 |
| 7:O:162:PRO:HB2 | 7:P:150:ALA:HA | 1.86 | 0.57 |
| 7:O:514:PRO:HG2 | 7:P:399:PHE:CD2 | 2.39 | 0.57 |
| 5:J:240:ASP:OD1 | 7:Q:4:ASN:ND2 | 2.38 | 0.57 |
| 9:T:104:LEU:O | 9:T:126:LEU:N | 2.31 | 0.57 |
| 1:X:502:ASN:N | 1:X:600:ASP:OD2 | 2.37 | 0.57 |
| 13:YA:320[C]:THR:HB | 13:YA:324[C]:ALA:HB2 | 1.85 | 0.57 |
| 13:YA:169[B]:ASP:HB2 | 13:YA:343[B]:VAL:HB | 1.86 | 0.57 |
| 13:YA:424[D]:VAL:HA | 13:YA:429[D]:ARG:O | 2.04 | 0.57 |
| 13:YA:424[F]:VAL:HA | 13:YA:429[F]:ARG:O | 2.04 | 0.57 |
| 13:YB:25[A]:GLY:HA3 | 13:YB:73[A]:VAL:HG12 | 1.86 | 0.57 |
| 13:YB:320[F]:THR:HB | 13:YB:324[F]:ALA:HB2 | 1.85 | 0.57 |
| 13:YA:399[B]:HIS:CD2 | 13:YB:403[B]:PHE:HB3 | 2.39 | 0.57 |
| 13:YB:567[E]:ILE:HG23 | 13:YC:565[E]:TYR:CE2 | 2.39 | 0.57 |
| 13:YC:424[A]:VAL:HA | 13:YC:429[A]:ARG:O | 2.04 | 0.57 |
| 13:YB:474[D]:ILE:HG12 | 13:YC:466[D]:ASN:HB2 | 1.85 | 0.57 |
| 13:YB:567[A]:ILE:HG23 | 13:YC:565[A]:TYR:CE2 | 2.38 | 0.57 |
| 13:YC:87[B]:LEU:HD21 | 13:YC:95[B]:ILE:HG23 | 1.85 | 0.57 |
| 14:YD:70[A]:ILE:HG21 | 14:YD:109[A]:LEU:HD21 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:349[B]:ASN:OD1 | 14:YD:350[B]:ASN:N | 2.38 | 0.57 |
| 14:YD:349[F]:ASN:OD1 | 14:YD:350[F]:ASN:N | 2.38 | 0.57 |
| 14:YE:70[A]:ILE:HG21 | 14:YE:109[A]:LEU:HD21 | 1.86 | 0.57 |
| 2:Z:963:TYR:CD1 | 2:Z:964:PRO:HD2 | 2.39 | 0.57 |
| 6:AH:107:VAL:O | 6:AH:114:VAL:N | 2.37 | 0.57 |
| 1:B:460:ALA:HA | 1:B:631:VAL:HG12 | 1.87 | 0.57 |
| 7:BA:142:ILE:HG21 | 7:BA:157:THR:O | 2.04 | 0.57 |
| 9:BD:53:PHE:HA | 9:BD:84:TYR:CE2 | 2.39 | 0.57 |
| 12:BG:204:HIS:HB3 | 12:BG:210:PRO:HA | 1.86 | 0.57 |
| 1:BH:145:PHE:CB | 1:BH:169:GLN:HA | 2.32 | 0.57 |
| 1:BH:400:ASN:OD1 | 1:BH:401:LEU:N | 2.38 | 0.57 |
| 1:BH:400:ASN:H | 1:BI:341:THR:HG22 | 1.69 | 0.57 |
| 2:C:855:ILE:HG23 | 2:C:856:ASN:CG | 2.25 | 0.57 |
| 4:CC:40:ASN:HB3 | 4:CC:45:GLN:HG2 | 1.84 | 0.57 |
| 5:CF:162:VAL:O | 5:CG:253:GLN:HA | 2.05 | 0.57 |
| 5:CH:186:TYR:OH | 5:CH:190:ASN:O | 2.12 | 0.57 |
| 7:DD:142:ILE:HG21 | 7:DD:157:THR:O | 2.04 | 0.57 |
| 8:DE:53:PHE:CD2 | 8:DE:54:MET:HG2 | 2.39 | 0.57 |
| 12:DJ:22:PHE:HA | 12:DJ:203:LEU:HA | 1.86 | 0.57 |
| 12:DJ:177:TRP:CZ3 | 12:DJ:220:SER:HB3 | 2.38 | 0.57 |
| 3:E:170:PRO:HB3 | 3:E:188:TRP:CG | 2.40 | 0.57 |
| 1:EA:363:PHE:CG | 1:EA:636:ASP:HB2 | 2.40 | 0.57 |
| 2:EC:529:SER:O | 2:EC:531:ARG:HG3 | 2.04 | 0.57 |
| 2:EC:977:ILE:HD12 | 2:EC:981:GLN:HA | 1.85 | 0.57 |
| 3:EE:170:PRO:HB3 | 3:EE:188:TRP:CG | 2.40 | 0.57 |
| 5:EI:156:SER:HB3 | 5:EJ:154:ILE:HG12 | 1.87 | 0.57 |
| 5:EJ:193:VAL:HG13 | 5:EJ:199:GLU:HB3 | 1.86 | 0.57 |
| 5:EJ:49:TRP:HZ3 | 5:EJ:96:ARG:HD2 | 1.70 | 0.57 |
| 5:FA:328:LEU:HD12 | 5:FA:330:HIS:CD2 | 2.38 | 0.57 |
| 6:FB:192:THR:HB | 6:FB:219:ALA:HB3 | 1.87 | 0.57 |
| 7:FE:40:SER:HB3 | 7:FF:24:ASN:HB3 | 1.87 | 0.57 |
| 7:FE:96:GLY:N | 7:FG:97:LEU:HB3 | 2.19 | 0.57 |
| 7:FE:441:GLN:N | 7:FG:513:ARG:O | 2.35 | 0.57 |
| 8:FI:10:PHE:C | 8:FI:12:SER:H | 2.08 | 0.57 |
| 11:GB:88:THR:H | 11:GB:163:ASN:HD21 | 1.52 | 0.57 |
| 1:GD:544:ASP:HB2 | 1:GD:576:ASP:CG | 2.24 | 0.57 |
| 5:HB:36:GLU:HA | 5:HB:50:LYS:HZ1 | 1.68 | 0.57 |
| 6:HE:192:THR:HB | 6:HE:219:ALA:HB3 | 1.87 | 0.57 |
| 6:HE:58:ASP:OD1 | 6:HF:164:GLN:NE2 | 2.37 | 0.57 |
| 6:HE:13:ARG:HB2 | 6:HG:10:VAL:HA | 1.86 | 0.57 |
| 7:HH:43:GLY:O | 7:HI:42:ALA:HB3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:359:TRP:NE1 | 7:HJ:340:THR:O | 2.36 | 0.57 |
| 5:I:213:GLY:O | 5:I:214:SER:OG | 2.23 | 0.57 |
| 5:I:362:GLU:HG3 | 5:I:363:ASN:N | 2.17 | 0.57 |
| 12:IF:204:HIS:HB3 | 12:IF:210:PRO:HA | 1.86 | 0.57 |
| 5:J:44:TYR:CD2 | 5:J:48:ALA:HB2 | 2.37 | 0.57 |
| 5:J:501:LEU:HD13 | 5:J:512:PRO:HG2 | 1.87 | 0.57 |
| 5:K:339:GLU:HG2 | 6:L:173:THR:HB | 1.85 | 0.57 |
| 5:J:196:ARG:HE | 7:Q:5:THR:HG23 | 1.70 | 0.57 |
| 11:V:186:ARG:CG | 11:V:187:ILE:N | 2.68 | 0.57 |
| 1:X:60:LEU:HD22 | 2:Z:671:TYR:CE1 | 2.39 | 0.57 |
| 1:Y:524:VAL:HG12 | 1:Y:527:ASP:H | 1.68 | 0.57 |
| 13:YA:17[C]:ASP:OD1 | 13:YA:19[C]:MET:N | 2.38 | 0.57 |
| 13:YA:169[D]:ASP:HB2 | 13:YA:343[D]:VAL:HB | 1.85 | 0.57 |
| 13:YA:376[B]:PHE:CE2 | 13:YB:447[B]:ASN:HB3 | 2.40 | 0.57 |
| 13:YA:399[D]:HIS:CD2 | 13:YB:403[D]:PHE:HB3 | 2.39 | 0.57 |
| 13:YA:424[E]:VAL:HA | 13:YA:429[E]:ARG:O | 2.04 | 0.57 |
| 13:YB:25[B]:GLY:HA3 | 13:YB:73[B]:VAL:HG12 | 1.87 | 0.57 |
| 13:YB:424[B]:VAL:HA | 13:YB:429[B]:ARG:O | 2.04 | 0.57 |
| 13:YB:87[B]:LEU:HD21 | 13:YB:95[B]:ILE:HG23 | 1.85 | 0.57 |
| 13:YB:88[C]:ASP:OD1 | 13:YB:88[C]:ASP:N | 2.38 | 0.57 |
| 13:YC:424[F]:VAL:HA | 13:YC:429[F]:ARG:O | 2.04 | 0.57 |
| 13:YB:474[E]:ILE:HG12 | 13:YC:466[E]:ASN:HB2 | 1.86 | 0.57 |
| 13:YC:82[D]:VAL:HG22 | 13:YC:98[D]:GLY:O | 2.04 | 0.57 |
| 14:YD:35[D]:ILE:HD11 | 14:YD:38[D]:LEU:HB2 | 1.87 | 0.57 |
| 14:YE:349[D]:ASN:OD1 | 14:YE:350[D]:ASN:N | 2.38 | 0.57 |
| 14:YE:70[F]:ILE:HG21 | 14:YE:109[F]:LEU:HD21 | 1.85 | 0.57 |
| 14:YE:98[F]:ASP:OD1 | 14:YE:99[F]:SER:N | 2.38 | 0.57 |
| 14:YF:349[D]:ASN:OD1 | 14:YF:350[D]:ASN:N | 2.38 | 0.57 |
| 2:Z:855:ILE:HG23 | 2:Z:856:ASN:CG | 2.25 | 0.57 |
| 15:ZA:67[A]:VAL:HG21 | 15:ZA:96[A]:ILE:HB | 1.86 | 0.57 |
| 1:A:510:MET:HE3 | 1:A:623:LEU:HD11 | 1.87 | 0.57 |
| 1:A:544:ASP:HB2 | 1:A:576:ASP:CG | 2.24 | 0.57 |
| 4:AB:202:LEU:HB3 | 4:AB:278:VAL:HG22 | 1.86 | 0.57 |
| 5:AD:132:ASP:OD2 | 5:AD:151:ILE:N | 2.36 | 0.57 |
| 5:AC:255:ARG:NE | 5:AE:390:LEU:HD12 | 2.19 | 0.57 |
| 7:AJ:99:ARG:HD3 | 7:AJ:111:ASN:ND2 | 2.20 | 0.57 |
| 1:B:524:VAL:HG12 | 1:B:527:ASP:H | 1.69 | 0.57 |
| 7:AJ:447:HIS:HD2 | 7:BA:447:HIS:CD2 | 2.23 | 0.57 |
| 8:BB:53:PHE:CD2 | 8:BB:54:MET:HG2 | 2.39 | 0.57 |
| 1:BH:399:TYR:O | 1:BH:400:ASN:HB2 | 2.04 | 0.57 |
| 1:BH:484:MET:HE1 | 1:BH:501:TYR:HB3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:206:GLN:HG3 | 5:CH:555:CYS:O | 2.05 | 0.57 |
| 2:C:167:ILE:O | 2:C:168:ILE:HG22 | 2.05 | 0.57 |
| 2:C:340:PRO:HA | 2:C:345:TYR:HE1 | 1.68 | 0.57 |
| 2:C:909:THR:OG1 | 2:C:910:GLU:OE1 | 2.11 | 0.57 |
| 4:CC:171:LYS:HB2 | 4:CD:165:GLU:HB3 | 1.85 | 0.57 |
| 4:CE:239:ARG:HD2 | 4:CE:249:ILE:HD12 | 1.85 | 0.57 |
| 5:CG:213:GLY:O | 5:CG:214:SER:OG | 2.22 | 0.57 |
| 5:CH:291:ILE:HG22 | 5:CH:292:PRO:O | 2.04 | 0.57 |
| 3:D:48:SER:OG | 3:D:49:SER:N | 2.37 | 0.57 |
| 8:DF:53:PHE:CD2 | 8:DF:54:MET:HG2 | 2.39 | 0.57 |
| 11:DI:110:VAL:HG22 | 11:DI:111:TYR:HD2 | 1.68 | 0.57 |
| 12:DJ:216:PHE:CE1 | 12:DJ:218:MET:HE3 | 2.40 | 0.57 |
| 2:EC:855:ILE:HG23 | 2:EC:856:ASN:CG | 2.25 | 0.57 |
| 3:ED:116:SER:HA | 3:ED:128:TRP:NE1 | 2.20 | 0.57 |
| 5:EI:187:ASN:HB2 | 5:EI:254:TRP:CZ2 | 2.39 | 0.57 |
| 5:EI:419:ASP:OD1 | 5:EI:420:VAL:N | 2.37 | 0.57 |
| 5:EI:520:GLY:O | 5:FA:591:PRO:HA | 2.05 | 0.57 |
| 5:EJ:132:ASP:OD2 | 5:EJ:151:ILE:N | 2.36 | 0.57 |
| 5:EJ:139:ALA:HB3 | 5:FA:99:PHE:HB3 | 1.87 | 0.57 |
| 5:FA:469:PRO:HA | 5:FA:472:TYR:CE2 | 2.39 | 0.57 |
| 7:FE:192:GLN:NE2 | 7:FF:186:SER:O | 2.37 | 0.57 |
| 7:FG:466:SER:HB3 | 7:FG:468:PHE:HE2 | 1.68 | 0.57 |
| 9:FJ:98:VAL:HB | 9:FJ:103:THR:HB | 1.86 | 0.57 |
| 9:FJ:53:PHE:HA | 9:FJ:84:TYR:CE2 | 2.39 | 0.57 |
| 4:G:171:LYS:HB2 | 4:H:165:GLU:HB3 | 1.86 | 0.57 |
| 4:G:202:LEU:HB3 | 4:G:278:VAL:HG22 | 1.87 | 0.57 |
| 12:GC:144:ASN:ND2 | 10:ID:57:LEU:HG | 2.20 | 0.57 |
| 2:GF:304:VAL:HG13 | 2:GF:327:ARG:NH1 | 2.16 | 0.57 |
| 2:GF:168:ILE:HG12 | 2:GF:578:PHE:HZ | 1.69 | 0.57 |
| 2:GF:982:LEU:O | 2:GF:985:GLU:HB2 | 2.05 | 0.57 |
| 4:F:165:GLU:HB3 | 4:H:171:LYS:HB2 | 1.85 | 0.57 |
| 4:HA:202:LEU:HB3 | 4:HA:278:VAL:HG22 | 1.87 | 0.57 |
| 5:HB:213:GLY:HA2 | 5:HB:221:GLU:HB2 | 1.87 | 0.57 |
| 5:HB:469:PRO:HA | 5:HB:472:TYR:CE2 | 2.39 | 0.57 |
| 5:HB:569:TYR:CD1 | 5:HC:544:VAL:HA | 2.38 | 0.57 |
| 5:HB:71:ASN:OD1 | 5:HB:73:SER:N | 2.27 | 0.57 |
| 5:HC:501:LEU:HD13 | 5:HC:512:PRO:HG2 | 1.87 | 0.57 |
| 6:HF:107:VAL:O | 6:HF:114:VAL:N | 2.37 | 0.57 |
| 7:HI:233:GLN:HE21 | 7:HI:237:ASN:ND2 | 2.01 | 0.57 |
| 11:IE:40:LEU:HD21 | 11:IE:45:LEU:HD11 | 1.85 | 0.57 |
| 5:J:193:VAL:HG13 | 5:J:199:GLU:HB3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:206:PHE:HZ | 5:J:221:GLU:HG2 | 1.70 | 0.57 |
| 5:K:291:ILE:HG22 | 5:K:292:PRO:O | 2.05 | 0.57 |
| 5:K:320:LEU:HD23 | 5:K:358:VAL:HG23 | 1.87 | 0.57 |
| 5:K:490:TRP:NE1 | 5:K:515:THR:O | 2.36 | 0.57 |
| 6:M:107:VAL:O | 6:M:114:VAL:N | 2.37 | 0.57 |
| 5:I:356:TYR:CE1 | 6:N:4:LEU:HD13 | 2.38 | 0.57 |
| 6:L:12:SER:CB | 6:N:6:ASN:HB3 | 2.35 | 0.57 |
| 7:P:513:ARG:O | 7:Q:441:GLN:N | 2.22 | 0.57 |
| 7:Q:47:VAL:HA | 7:Q:57:ILE:HD12 | 1.85 | 0.57 |
| 12:W:233:ASP:HA | 12:IF:20:ASN:OD1 | 2.04 | 0.57 |
| 1:X:201:VAL:HG22 | 1:X:202:ASP:H | 1.70 | 0.57 |
| 1:Y:594:GLU:N | 1:Y:594:GLU:OE1 | 2.38 | 0.57 |
| 13:YA:320[B]:THR:HB | 13:YA:324[B]:ALA:HB2 | 1.84 | 0.57 |
| 13:YA:376[E]:PHE:CE2 | 13:YB:447[E]:ASN:HB3 | 2.40 | 0.57 |
| 13:YA:575[D]:GLY:N | 13:YB:567[D]:ILE:O | 2.37 | 0.57 |
| 13:YA:65[F]:ALA:N | 13:YA:69[F]:ILE:O | 2.36 | 0.57 |
| 13:YB:17[F]:ASP:OD1 | 13:YB:19[F]:MET:N | 2.38 | 0.57 |
| 13:YB:424[D]:VAL:HA | 13:YB:429[D]:ARG:O | 2.04 | 0.57 |
| 13:YB:61[D]:ILE:HA | 13:YC:76[D]:PRO:HA | 1.85 | 0.57 |
| 13:YC:169[F]:ASP:HB2 | 13:YC:343[F]:VAL:HB | 1.86 | 0.57 |
| 13:YC:88[D]:ASP:N | 13:YC:88[D]:ASP:OD1 | 2.38 | 0.57 |
| 14:YD:349[A]:ASN:OD1 | 14:YD:350[A]:ASN:N | 2.38 | 0.57 |
| 14:YD:349[C]:ASN:OD1 | 14:YD:350[C]:ASN:N | 2.38 | 0.57 |
| 14:YE:349[A]:ASN:OD1 | 14:YE:350[A]:ASN:N | 2.38 | 0.57 |
| 14:YE:349[F]:ASN:OD1 | 14:YE:350[F]:ASN:N | 2.38 | 0.57 |
| 11:BF:190:LYS:HE3 | 14:YF:24[F]:SER:O | 2.05 | 0.57 |
| 14:YF:349[C]:ASN:OD1 | 14:YF:350[C]:ASN:N | 2.38 | 0.57 |
| 2:Z:167:ILE:O | 2:Z:168:ILE:HG22 | 2.05 | 0.57 |
| 2:Z:41:THR:HG1 | 2:Z:77:THR:HG1 | 1.35 | 0.57 |
| 2:Z:929:TYR:CZ | 2:Z:963:TYR:HD1 | 2.22 | 0.57 |
| 5:AC:213:GLY:HA2 | 5:AC:221:GLU:HB2 | 1.87 | 0.57 |
| 5:AD:164:ARG:HG3 | 5:AD:245:GLU:HG2 | 1.86 | 0.57 |
| 5:AD:71:ASN:OD1 | 5:AD:73:SER:N | 2.23 | 0.57 |
| 6:AF:107:VAL:O | 6:AF:114:VAL:N | 2.37 | 0.57 |
| 7:AI:440:GLN:OE1 | 7:AI:511:GLU:HG3 | 2.05 | 0.57 |
| 1:B:496:GLU:HG3 | 2:C:856:ASN:O | 2.04 | 0.57 |
| 1:BH:363:PHE:CG | 1:BH:636:ASP:HB2 | 2.40 | 0.57 |
| 2:BJ:1012:LEU:HD13 | 2:BJ:1027:GLN:OE1 | 2.05 | 0.57 |
| 2:BJ:929:TYR:CD2 | 2:BJ:961:VAL:HB | 2.39 | 0.57 |
| 4:CC:141:SER:HB3 | 4:CC:164:ILE:HD11 | 1.87 | 0.57 |
| 4:CD:239:ARG:HD2 | 4:CD:249:ILE:HD12 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CE:141:SER:HB3 | 4:CE:164:ILE:HD11 | 1.87 | 0.57 |
| 4:CE:42:PHE:O | 4:CE:62:HIS:ND1 | 2.27 | 0.57 |
| 5:CG:132:ASP:OD2 | 5:CG:151:ILE:N | 2.36 | 0.57 |
| 5:CG:136:VAL:O | 5:CG:143:TRP:HA | 2.04 | 0.57 |
| 5:CH:89:TYR:O | 5:CH:91:LYS:HG2 | 2.04 | 0.57 |
| 3:D:116:SER:HA | 3:D:128:TRP:NE1 | 2.19 | 0.57 |
| 3:D:46:PRO:HG3 | 3:D:270:ARG:HH22 | 1.68 | 0.57 |
| 7:DB:130:GLU:HA | 7:DC:139:ASN:HD21 | 1.69 | 0.57 |
| 7:DB:184:THR:OG1 | 7:DB:187:ASP:N | 2.34 | 0.57 |
| 7:DC:118:PRO:HA | 7:DC:121:PHE:HB3 | 1.86 | 0.57 |
| 7:DC:44:VAL:HG21 | 7:DD:25:PHE:HB3 | 1.87 | 0.57 |
| 7:DC:447:HIS:HD2 | 7:DD:447:HIS:CD2 | 2.22 | 0.57 |
| 3:E:175:ASP:OD2 | 2:GF:509:TYR:HB2 | 2.05 | 0.57 |
| 3:D:9:ARG:HD2 | 3:E:60:TYR:HD1 | 1.68 | 0.57 |
| 1:EB:111:MET:HB3 | 1:EB:164:ARG:HG2 | 1.86 | 0.57 |
| 1:EB:83:ALA:O | 1:EB:326:ARG:NH2 | 2.36 | 0.57 |
| 2:EC:768:TYR:OH | 2:EC:814:HIS:O | 2.17 | 0.57 |
| 2:EC:814:HIS:HB2 | 2:EC:862:TYR:HE1 | 1.69 | 0.57 |
| 2:EC:929:TYR:CZ | 2:EC:963:TYR:HD1 | 2.22 | 0.57 |
| 3:ED:130:VAL:HG12 | 3:ED:191:LEU:HD12 | 1.86 | 0.57 |
| 3:ED:9:ARG:HD2 | 3:EE:60:TYR:HD1 | 1.68 | 0.57 |
| 4:EF:166:SER:H | 4:EH:172:GLU:HA | 1.70 | 0.57 |
| 4:EH:42:PHE:O | 4:EH:62:HIS:ND1 | 2.27 | 0.57 |
| 5:EJ:164:ARG:HG3 | 5:EJ:245:GLU:HG2 | 1.86 | 0.57 |
| 5:EJ:419:ASP:HB3 | 5:EJ:436:VAL:HB | 1.86 | 0.57 |
| 6:CI:75:THR:HB | 7:FF:167:GLN:NE2 | 2.19 | 0.57 |
| 7:FF:509:GLY:HA3 | 7:FG:441:GLN:NE2 | 2.20 | 0.57 |
| 1:GD:400:ASN:OD1 | 1:GD:401:LEU:N | 2.38 | 0.57 |
| 1:GE:174:ARG:NH2 | 1:GE:269:VAL:HG21 | 2.18 | 0.57 |
| 2:GF:189:ARG:HG2 | 2:GF:204:ARG:HH12 | 1.69 | 0.57 |
| 4:HA:46:ARG:NH2 | 4:HA:66:TYR:OH | 2.36 | 0.57 |
| 5:HB:419:ASP:OD1 | 5:HB:420:VAL:N | 2.37 | 0.57 |
| 5:HC:164:ARG:HG3 | 5:HC:245:GLU:HG2 | 1.86 | 0.57 |
| 5:HC:569:TYR:OH | 5:HD:571:GLU:OE2 | 2.09 | 0.57 |
| 7:HH:440:GLN:OE1 | 7:HH:511:GLU:HG3 | 2.04 | 0.57 |
| 7:HJ:49:ASP:HA | 7:HJ:57:ILE:O | 2.05 | 0.57 |
| 11:IE:186:ARG:CG | 11:IE:187:ILE:N | 2.68 | 0.57 |
| 12:IF:177:TRP:CZ3 | 12:IF:220:SER:HB3 | 2.38 | 0.57 |
| 5:J:73:SER:HB3 | 5:J:101:THR:HG21 | 1.87 | 0.57 |
| 5:J:150:GLN:HB2 | 5:J:152:ASP:HB3 | 1.84 | 0.57 |
| 5:I:162:VAL:O | 5:J:253:GLN:HA | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:507:ASP:OD1 | 5:K:511:ASN:N | 2.25 | 0.57 |
| 7:O:375:TYR:HE2 | 7:O:390:PRO:HB2 | 1.69 | 0.57 |
| 7:P:77:THR:HG23 | 7:P:79:ALA:N | 2.19 | 0.57 |
| 10:U:39:PRO:HG3 | 10:U:42:ARG:HH21 | 1.69 | 0.57 |
| 12:W:157:PRO:HD3 | 12:IF:137:TYR:OH | 2.03 | 0.57 |
| 1:X:555:ILE:O | 1:X:589:TYR:HD1 | 1.87 | 0.57 |
| 1:Y:363:PHE:CD1 | 1:Y:636:ASP:HB2 | 2.39 | 0.57 |
| 1:Y:452:VAL:O | 1:Y:457:SER:OG | 2.22 | 0.57 |
| 13:YA:17[F]:ASP:OD1 | 13:YA:19[F]:MET:N | 2.38 | 0.57 |
| 13:YA:57[A]:VAL:CG1 | 13:YA:76[A]:PRO:HD3 | 2.34 | 0.57 |
| 13:YA:61[D]:ILE:HD11 | 13:YB:72[D]:SER:O | 2.03 | 0.57 |
| 13:YA:76[A]:PRO:C | 13:YC:61[A]:ILE:HA | 2.25 | 0.57 |
| 13:YA:82[A]:VAL:HG22 | 13:YA:98[A]:GLY:O | 2.04 | 0.57 |
| 13:YA:522[E]:VAL:HA | 13:YB:514[E]:VAL:O | 2.05 | 0.57 |
| 13:YC:25[A]:GLY:HA3 | 13:YC:73[A]:VAL:HG12 | 1.86 | 0.57 |
| 13:YC:169[A]:ASP:HB2 | 13:YC:343[A]:VAL:HB | 1.85 | 0.57 |
| 13:YA:83[D]:TYR:CZ | 13:YC:95[D]:ILE:HD11 | 2.39 | 0.57 |
| 14:YD:64[A]:MET:HE3 | 14:YD:68[A]:GLU:HG3 | 1.87 | 0.57 |
| 14:YD:98[F]:ASP:OD1 | 14:YD:99[F]:SER:N | 2.38 | 0.57 |
| 14:YE:349[B]:ASN:OD1 | 14:YE:350[B]:ASN:N | 2.38 | 0.57 |
| 14:YE:98[E]:ASP:OD1 | 14:YE:99[E]:SER:N | 2.38 | 0.57 |
| 14:YD:61[E]:HIS:CE1 | 14:YF:332[E]:GLN:HB3 | 2.38 | 0.57 |
| 2:Z:724:ALA:O | 2:Z:726:PHE:N | 2.36 | 0.57 |
| 5:AD:200:LEU:HD22 | 7:AJ:2:SER:HA | 1.87 | 0.57 |
| 5:AE:313:PHE:CE2 | 5:AE:320:LEU:HD21 | 2.39 | 0.57 |
| 11:BF:186:ARG:CG | 11:BF:187:ILE:N | 2.68 | 0.57 |
| 1:BH:201:VAL:HG22 | 1:BH:202:ASP:H | 1.70 | 0.57 |
| 1:BH:431:GLU:HG2 | 1:BH:435:TRP:CE3 | 2.38 | 0.57 |
| 2:C:246:TYR:HE1 | 2:C:255:TYR:HD1 | 1.51 | 0.57 |
| 2:C:555:ARG:HG3 | 2:C:557:VAL:H | 1.68 | 0.57 |
| 5:CF:469:PRO:HA | 5:CF:472:TYR:CE2 | 2.39 | 0.57 |
| 5:CF:255:ARG:NE | 5:CH:390:LEU:HD12 | 2.20 | 0.57 |
| 5:CG:139:ALA:HB3 | 5:CH:99:PHE:HB3 | 1.85 | 0.57 |
| 7:DB:422:LYS:HB3 | 7:DC:504:ARG:HA | 1.87 | 0.57 |
| 7:DD:466:SER:HB3 | 7:DD:468:PHE:HE2 | 1.68 | 0.57 |
| 1:EB:524:VAL:HG12 | 1:EB:527:ASP:H | 1.68 | 0.57 |
| 5:EJ:131:SER:HA | 5:EJ:150:GLN:HA | 1.85 | 0.57 |
| 5:EJ:136:VAL:O | 5:EJ:143:TRP:HA | 2.04 | 0.57 |
| 5:EJ:501:LEU:HD13 | 5:EJ:512:PRO:HG2 | 1.87 | 0.57 |
| 4:F:141:SER:HB3 | 4:F:164:ILE:HD11 | 1.87 | 0.57 |
| 4:F:40:ASN:HB3 | 4:F:45:GLN:HG2 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:563:GLY:O | 5:FA:565:ILE:N | 2.34 | 0.57 |
| 6:FD:107:VAL:O | 6:FD:114:VAL:N | 2.37 | 0.57 |
| 7:FG:466:SER:HB3 | 7:FG:468:PHE:CE2 | 2.40 | 0.57 |
| 4:G:40:ASN:HB3 | 4:G:45:GLN:HG2 | 1.84 | 0.57 |
| 1:GD:145:PHE:CB | 1:GD:169:GLN:HA | 2.32 | 0.57 |
| 1:GD:431:GLU:HG2 | 1:GD:435:TRP:CE3 | 2.39 | 0.57 |
| 1:GD:494:THR:HG21 | 1:GD:603:TYR:HA | 1.86 | 0.57 |
| 1:GD:555:ILE:O | 1:GD:589:TYR:HD1 | 1.87 | 0.57 |
| 2:GF:146:LEU:HD13 | 2:GF:582:ALA:HB1 | 1.87 | 0.57 |
| 2:GF:167:ILE:O | 2:GF:168:ILE:HG22 | 2.05 | 0.57 |
| 2:GF:376:PHE:CB | 2:GF:405:VAL:HA | 2.35 | 0.57 |
| 2:GF:855:ILE:HG23 | 2:GF:856:ASN:CG | 2.25 | 0.57 |
| 5:HB:156:SER:HB3 | 5:HC:154:ILE:HG12 | 1.87 | 0.57 |
| 5:HC:200:LEU:HD22 | 7:HI:2:SER:HA | 1.87 | 0.57 |
| 5:HC:247:PHE:HZ | 5:HD:162:VAL:HG21 | 1.70 | 0.57 |
| 5:HD:237:ASN:OD1 | 5:HD:238:ILE:N | 2.38 | 0.57 |
| 5:HD:270:LEU:HG | 6:HG:108:LEU:HD21 | 1.87 | 0.57 |
| 6:HE:107:VAL:O | 6:HE:114:VAL:N | 2.38 | 0.57 |
| 6:HF:69:THR:HA | 6:HG:73:ASN:HB3 | 1.87 | 0.57 |
| 7:HI:192:GLN:NE2 | 7:HJ:185:GLU:O | 2.33 | 0.57 |
| 7:HH:199:VAL:HG12 | 7:HJ:212:PRO:HG3 | 1.87 | 0.57 |
| 8:IA:14:ASP:OD2 | 8:IA:17:ARG:NH2 | 2.33 | 0.57 |
| 10:ID:39:PRO:HG3 | 10:ID:42:ARG:HH21 | 1.69 | 0.57 |
| 6:N:192:THR:HB | 6:N:219:ALA:HB3 | 1.87 | 0.57 |
| 8:S:27:TYR:HD2 | 8:S:28:LEU:HD12 | 1.69 | 0.57 |
| 1:X:423:THR:O | 1:X:476:ILE:N | 2.35 | 0.57 |
| 13:YA:193[B]:ASP:OD1 | 13:YA:197[B]:TYR:N | 2.32 | 0.57 |
| 13:YA:376[C]:PHE:CE2 | 13:YB:447[C]:ASN:HB3 | 2.40 | 0.57 |
| 13:YA:399[E]:HIS:CD2 | 13:YB:403[E]:PHE:HB3 | 2.39 | 0.57 |
| 13:YA:50[D]:GLU:N | 13:YA:50[D]:GLU:OE2 | 2.33 | 0.57 |
| 13:YA:60[F]:PRO:HD2 | 13:YC:61[F]:ILE:HG12 | 1.86 | 0.57 |
| 13:YA:25[A]:GLY:HA3 | 13:YA:73[A]:VAL:HG12 | 1.86 | 0.57 |
| 13:YA:88[A]:ASP:OD1 | 13:YA:88[A]:ASP:N | 2.38 | 0.57 |
| 13:YB:17[C]:ASP:OD1 | 13:YB:19[C]:MET:N | 2.38 | 0.57 |
| 13:YB:416[A]:HIS:HD2 | 13:YB:418[A]:THR:H | 1.51 | 0.57 |
| 13:YB:424[C]:VAL:HA | 13:YB:429[C]:ARG:O | 2.04 | 0.57 |
| 13:YB:47[E]:ILE:HG23 | 14:YE:123[E]:PRO:CG | 2.30 | 0.57 |
| 13:YB:567[B]:ILE:HG23 | 13:YC:565[B]:TYR:CE2 | 2.39 | 0.57 |
| 13:YB:87[F]:LEU:HD21 | 13:YB:95[F]:ILE:HG23 | 1.86 | 0.57 |
| 11:GB:190:LYS:HE3 | 14:YE:24[D]:SER:O | 2.04 | 0.57 |
| 14:YE:349[E]:ASN:OD1 | 14:YE:350[E]:ASN:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:98[A]:ASP:OD1 | 14:YE:99[A]:SER:N | 2.38 | 0.57 |
| 14:YF:349[F]:ASN:OD1 | 14:YF:350[F]:ASN:N | 2.38 | 0.57 |
| 2:Z:154:SER:OG | 2:Z:156:SER:OG | 2.13 | 0.57 |
| 2:Z:182:GLN:O | 2:Z:210:LYS:NZ | 2.33 | 0.57 |
| 2:Z:19:ASN:OD1 | 2:Z:20:GLN:HG3 | 2.05 | 0.57 |
| 2:C:581:TYR:OH | 2:Z:850:ASN:HB3 | 2.05 | 0.57 |
| 2:Z:848:LEU:O | 2:Z:850:ASN:N | 2.37 | 0.57 |
| 4:AB:141:SER:HB3 | 4:AB:164:ILE:HD11 | 1.87 | 0.57 |
| 5:AC:213:GLY:O | 5:AC:214:SER:OG | 2.23 | 0.57 |
| 5:AC:30:PHE:HE1 | 5:AE:30:PHE:CE1 | 2.23 | 0.57 |
| 5:AE:237:ASN:OD1 | 5:AE:238:ILE:N | 2.38 | 0.57 |
| 5:AE:320:LEU:HD23 | 5:AE:358:VAL:HG23 | 1.87 | 0.57 |
| 1:B:594:GLU:OE1 | 1:B:594:GLU:N | 2.38 | 0.57 |
| 1:B:363:PHE:CD1 | 1:B:636:ASP:HB2 | 2.39 | 0.57 |
| 1:BI:111:MET:HB3 | 1:BI:164:ARG:HG2 | 1.86 | 0.57 |
| 1:BI:70:PHE:HE2 | 2:BJ:686:LEU:CB | 2.15 | 0.57 |
| 2:BJ:125:GLU:HG2 | 2:BJ:134:TYR:CD1 | 2.40 | 0.57 |
| 2:BJ:435:SER:HB3 | 2:BJ:512:PRO:HA | 1.86 | 0.57 |
| 2:BJ:855:ILE:HG23 | 2:BJ:856:ASN:CG | 2.25 | 0.57 |
| 2:BJ:814:HIS:HB2 | 2:BJ:862:TYR:HE1 | 1.69 | 0.57 |
| 2:BJ:992:PRO:HB3 | 5:CH:19:LEU:HB3 | 1.86 | 0.57 |
| 2:C:19:ASN:OD1 | 2:C:20:GLN:HG3 | 2.05 | 0.57 |
| 2:C:982:LEU:O | 2:C:985:GLU:HB2 | 2.05 | 0.57 |
| 3:CA:114:CYS:HA | 3:CA:120:ASN:OD1 | 2.05 | 0.57 |
| 4:CE:202:LEU:HB3 | 4:CE:278:VAL:HG22 | 1.86 | 0.57 |
| 5:CG:164:ARG:HG3 | 5:CG:245:GLU:HG2 | 1.86 | 0.57 |
| 5:CG:206:PHE:HZ | 5:CG:221:GLU:HG2 | 1.70 | 0.57 |
| 5:CG:318:GLN:HE22 | 6:CI:8:ALA:N | 2.01 | 0.57 |
| 6:DA:107:VAL:O | 6:DA:114:VAL:N | 2.37 | 0.57 |
| 7:DB:118:PRO:HG3 | 7:DC:106:ALA:HA | 1.87 | 0.57 |
| 10:DH:129:LEU:HD13 | 10:DH:209:TRP:HZ3 | 1.70 | 0.57 |
| 10:DH:237:THR:HA | 10:DH:287:VAL:HG23 | 1.87 | 0.57 |
| 11:DI:40:LEU:HD21 | 11:DI:45:LEU:HD11 | 1.85 | 0.57 |
| 1:EA:201:VAL:HG22 | 1:EA:202:ASP:H | 1.70 | 0.57 |
| 1:EA:60:LEU:HD22 | 2:EC:671:TYR:CD1 | 2.40 | 0.57 |
| 1:EA:619:GLN:N | 1:EA:619:GLN:OE1 | 2.36 | 0.57 |
| 1:EB:594:GLU:OE1 | 1:EB:594:GLU:N | 2.38 | 0.57 |
| 2:EC:98:GLU:N | 2:EC:98:GLU:OE1 | 2.30 | 0.57 |
| 4:EH:202:LEU:HB3 | 4:EH:278:VAL:HG22 | 1.86 | 0.57 |
| 5:EI:469:PRO:HA | 5:EI:472:TYR:CE2 | 2.40 | 0.57 |
| 5:FA:89:TYR:O | 5:FA:91:LYS:HG2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FG:49:ASP:HA | 7:FG:57:ILE:O | 2.05 | 0.57 |
| 4:G:36:ASN:OD1 | 4:H:7:LYS:NZ | 2.29 | 0.57 |
| 10:GA:237:THR:HA | 10:GA:287:VAL:HG23 | 1.87 | 0.57 |
| 12:DJ:20:ASN:OD1 | 12:GC:233:ASP:HA | 2.04 | 0.57 |
| 1:GD:399:TYR:O | 1:GD:400:ASN:HB2 | 2.04 | 0.57 |
| 2:GF:522:THR:HG22 | 2:GF:536:TYR:HB3 | 1.86 | 0.57 |
| 2:GF:781:LEU:HB2 | 2:GF:798:ILE:HD11 | 1.86 | 0.57 |
| 2:GF:963:TYR:CD1 | 2:GF:964:PRO:HD2 | 2.39 | 0.57 |
| 3:GH:90:ILE:HG23 | 3:GH:210:VAL:HG21 | 1.87 | 0.57 |
| 5:HB:162:VAL:O | 5:HC:253:GLN:HA | 2.05 | 0.57 |
| 5:HB:362:GLU:HG3 | 5:HB:363:ASN:N | 2.17 | 0.57 |
| 5:HB:36:GLU:HA | 5:HB:50:LYS:NZ | 2.20 | 0.57 |
| 7:HH:514:PRO:HB3 | 7:HI:512:THR:O | 2.04 | 0.57 |
| 7:HJ:9:VAL:HG23 | 7:HJ:10:SER:N | 2.20 | 0.57 |
| 5:I:156:SER:HB3 | 5:J:154:ILE:HG12 | 1.87 | 0.57 |
| 11:IE:88:THR:H | 11:IE:163:ASN:HD21 | 1.53 | 0.57 |
| 5:J:290:SER:CB | 5:J:370:HIS:HA | 2.35 | 0.57 |
| 5:J:49:TRP:HZ3 | 5:J:96:ARG:HD2 | 1.70 | 0.57 |
| 5:K:89:TYR:O | 5:K:91:LYS:HG2 | 2.04 | 0.57 |
| 7:O:514:PRO:HB3 | 7:P:512:THR:O | 2.05 | 0.57 |
| 8:R:55:ASN:HB3 | 8:BB:99:ILE:HD11 | 1.86 | 0.57 |
| 8:R:89:GLN:HB3 | 8:R:134:PRO:HG2 | 1.85 | 0.57 |
| 1:Y:209:TRP:HE3 | 1:Y:212:LYS:HB2 | 1.69 | 0.57 |
| 1:X:338:ARG:NH2 | 1:Y:340:VAL:O | 2.38 | 0.57 |
| 13:YA:575[E]:GLY:N | 13:YB:567[E]:ILE:O | 2.37 | 0.57 |
| 13:YB:61[A]:ILE:HA | 13:YC:76[A]:PRO:HA | 1.85 | 0.57 |
| 13:YB:61[F]:ILE:HG13 | 13:YB:62[F]:THR:N | 2.17 | 0.57 |
| 13:YA:76[D]:PRO:C | 13:YC:61[D]:ILE:HA | 2.25 | 0.57 |
| 14:YD:70[B]:ILE:HG21 | 14:YD:109[B]:LEU:HD21 | 1.86 | 0.57 |
| 14:YD:349[D]:ASN:OD1 | 14:YD:350[D]:ASN:N | 2.38 | 0.57 |
| 14:YE:35[D]:ILE:HD11 | 14:YE:38[D]:LEU:HB2 | 1.87 | 0.57 |
| 14:YF:349[E]:ASN:OD1 | 14:YF:350[E]:ASN:N | 2.38 | 0.57 |
| 14:YF:35[C]:ILE:HD11 | 14:YF:38[C]:LEU:HB2 | 1.87 | 0.57 |
| 14:YF:35[D]:ILE:HD11 | 14:YF:38[D]:LEU:HB2 | 1.87 | 0.57 |
| 2:Z:246:TYR:HE1 | 2:Z:255:TYR:HD1 | 1.51 | 0.57 |
| 1:A:494:THR:HG21 | 1:A:603:TYR:HA | 1.86 | 0.57 |
| 4:AB:46:ARG:NH2 | 4:AB:66:TYR:OH | 2.36 | 0.57 |
| 5:AC:60:LEU:HG | 5:AC:79:ILE:HG22 | 1.87 | 0.57 |
| 5:AD:129:ARG:HG3 | 5:AD:130:PHE:H | 1.70 | 0.57 |
| 1:B:102:SER:H | 1:B:194:ARG:NH1 | 2.02 | 0.57 |
| 7:AI:140:GLY:HA2 | 7:BA:129:PHE:HZ | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BA:466:SER:HB3 | 7:BA:468:PHE:CE2 | 2.40 | 0.57 |
| 7:BA:9:VAL:HG23 | 7:BA:10:SER:N | 2.20 | 0.57 |
| 9:BD:104:LEU:O | 9:BD:126:LEU:N | 2.31 | 0.57 |
| 12:BG:217:THR:O | 12:BG:246:ARG:N | 2.32 | 0.57 |
| 1:BI:594:GLU:OE1 | 1:BI:594:GLU:N | 2.38 | 0.57 |
| 2:BJ:19:ASN:OD1 | 2:BJ:20:GLN:HG3 | 2.05 | 0.57 |
| 2:BJ:929:TYR:CZ | 2:BJ:963:TYR:HD1 | 2.22 | 0.57 |
| 2:BJ:982:LEU:O | 2:BJ:985:GLU:HB2 | 2.05 | 0.57 |
| 2:C:376:PHE:CB | 2:C:405:VAL:HA | 2.35 | 0.57 |
| 2:C:435:SER:HB3 | 2:C:512:PRO:HA | 1.86 | 0.57 |
| 2:C:848:LEU:O | 2:C:850:ASN:N | 2.37 | 0.57 |
| 3:CB:104:TYR:HB3 | 3:CB:165:ARG:HB2 | 1.87 | 0.57 |
| 3:CB:219:ASP:OD1 | 3:CB:221:THR:N | 2.32 | 0.57 |
| 5:CG:49:TRP:HZ3 | 5:CG:96:ARG:HD2 | 1.70 | 0.57 |
| 5:CG:501:LEU:HD13 | 5:CG:512:PRO:HG2 | 1.87 | 0.57 |
| 5:CH:237:ASN:OD1 | 5:CH:238:ILE:N | 2.38 | 0.57 |
| 5:CH:563:GLY:O | 5:CH:565:ILE:N | 2.35 | 0.57 |
| 7:DB:72:ASN:HA | 7:DD:77:THR:HG21 | 1.87 | 0.57 |
| 7:DB:55:LYS:HB3 | 7:DD:57:ILE:HG22 | 1.85 | 0.57 |
| 3:E:176:ALA:HB1 | 2:GF:506:MET:HB3 | 1.87 | 0.57 |
| 3:E:177:GLU:HG3 | 3:E:180:ILE:HG22 | 1.86 | 0.57 |
| 1:EA:555:ILE:O | 1:EA:589:TYR:HD1 | 1.87 | 0.57 |
| 2:EC:296:THR:OG1 | 2:EC:298:ALA:O | 2.23 | 0.57 |
| 2:EC:982:LEU:O | 2:EC:985:GLU:HB2 | 2.05 | 0.57 |
| 3:EE:104:TYR:HB3 | 3:EE:165:ARG:HB2 | 1.87 | 0.57 |
| 3:EE:90:ILE:HG23 | 3:EE:210:VAL:HG21 | 1.87 | 0.57 |
| 4:EF:141:SER:HB3 | 4:EF:164:ILE:HD11 | 1.87 | 0.57 |
| 4:EH:141:SER:HB3 | 4:EH:164:ILE:HD11 | 1.87 | 0.57 |
| 5:EI:213:GLY:HA2 | 5:EI:221:GLU:HB2 | 1.87 | 0.57 |
| 7:FF:97:LEU:HB3 | 7:FG:95:TYR:HB3 | 1.85 | 0.57 |
| 7:FF:192:GLN:NE2 | 7:FG:185:GLU:O | 2.34 | 0.57 |
| 11:GB:186:ARG:CG | 11:GB:187:ILE:N | 2.68 | 0.57 |
| 1:GD:201:VAL:HG22 | 1:GD:202:ASP:H | 1.70 | 0.57 |
| 1:GD:484:MET:HE1 | 1:GD:501:TYR:HB3 | 1.87 | 0.57 |
| 2:GF:1000:THR:HG22 | 2:GF:1001:PHE:H | 1.70 | 0.57 |
| 5:HB:49:TRP:C | 5:HD:90:ASN:HD21 | 2.06 | 0.57 |
| 5:HD:89:TYR:O | 5:HD:91:LYS:HG2 | 2.04 | 0.57 |
| 6:HE:13:ARG:NH1 | 6:HG:17:PHE:O | 2.30 | 0.57 |
| 7:HJ:54:THR:HG22 | 7:HJ:55:LYS:O | 2.05 | 0.57 |
| 5:I:469:PRO:HA | 5:I:472:TYR:CE2 | 2.39 | 0.57 |
| 5:I:36:GLU:HA | 5:I:50:LYS:NZ | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:IB:10:PHE:C | 8:IB:12:SER:H | 2.08 | 0.57 |
| 10:ID:285:LEU:HA | 14:YF:215[B]:GLU:HG3 | 1.86 | 0.57 |
| 5:J:129:ARG:HG3 | 5:J:130:PHE:H | 1.70 | 0.57 |
| 7:O:43:GLY:O | 7:P:42:ALA:HB3 | 2.05 | 0.57 |
| 1:Y:184:PRO:HB2 | 1:Y:186:ILE:HD11 | 1.86 | 0.57 |
| 13:YA:88[B]:ASP:OD1 | 13:YA:88[B]:ASP:N | 2.38 | 0.57 |
| 13:YB:169[C]:ASP:HB2 | 13:YB:343[C]:VAL:HB | 1.86 | 0.57 |
| 13:YB:416[E]:HIS:HD2 | 13:YB:418[E]:THR:H | 1.52 | 0.57 |
| 13:YA:522[F]:VAL:HA | 13:YB:514[F]:VAL:O | 2.05 | 0.57 |
| 13:YB:82[E]:VAL:HG22 | 13:YB:98[E]:GLY:O | 2.05 | 0.57 |
| 13:YB:88[E]:ASP:N | 13:YB:88[E]:ASP:OD1 | 2.37 | 0.57 |
| 13:YB:88[F]:ASP:OD1 | 13:YB:88[F]:ASP:N | 2.38 | 0.57 |
| 13:YC:17[F]:ASP:OD1 | 13:YC:19[F]:MET:N | 2.38 | 0.57 |
| 13:YC:193[D]:ASP:OD1 | 13:YC:197[D]:TYR:N | 2.33 | 0.57 |
| 13:YC:88[E]:ASP:OD1 | 13:YC:88[E]:ASP:N | 2.37 | 0.57 |
| 13:YC:88[C]:ASP:N | 13:YC:88[C]:ASP:OD1 | 2.38 | 0.57 |
| 14:YE:349[C]:ASN:OD1 | 14:YE:350[C]:ASN:N | 2.38 | 0.57 |
| 14:YE:35[B]:ILE:HD11 | 14:YE:38[B]:LEU:HB2 | 1.87 | 0.57 |
| 14:YE:35[C]:ILE:HD11 | 14:YE:38[C]:LEU:HB2 | 1.87 | 0.57 |
| 14:YE:64[F]:MET:HE3 | 14:YE:68[F]:GLU:HG3 | 1.87 | 0.57 |
| 14:YF:349[A]:ASN:OD1 | 14:YF:350[A]:ASN:N | 2.38 | 0.57 |
| 14:YF:98[E]:ASP:OD1 | 14:YF:99[E]:SER:N | 2.38 | 0.57 |
| 2:Z:1000:THR:HG22 | 2:Z:1001:PHE:H | 1.70 | 0.57 |
| 2:Z:1012:LEU:HD13 | 2:Z:1027:GLN:OE1 | 2.05 | 0.57 |
| 2:Z:793:CYS:HB3 | 2:Z:813:ILE:HG12 | 1.87 | 0.57 |
| 1:A:112:LEU:HB2 | 1:A:300:ILE:HG22 | 1.86 | 0.57 |
| 1:A:363:PHE:CG | 1:A:636:ASP:HB2 | 2.39 | 0.57 |
| 4:AA:202:LEU:HB3 | 4:AA:278:VAL:HG22 | 1.86 | 0.57 |
| 5:AC:34:TYR:O | 5:AC:38:GLY:N | 2.26 | 0.57 |
| 5:AC:36:GLU:HA | 5:AC:50:LYS:NZ | 2.20 | 0.57 |
| 5:AD:501:LEU:HD13 | 5:AD:512:PRO:HG2 | 1.87 | 0.57 |
| 5:AE:291:ILE:HG22 | 5:AE:292:PRO:O | 2.05 | 0.57 |
| 5:AD:569:TYR:OH | 5:AE:571:GLU:OE2 | 2.14 | 0.57 |
| 6:AG:192:THR:HB | 6:AG:219:ALA:HB3 | 1.87 | 0.57 |
| 7:AJ:71:ASN:CB | 7:DD:365:GLY:HA2 | 2.35 | 0.57 |
| 1:B:229:THR:OG1 | 1:B:233:ASN:O | 2.23 | 0.57 |
| 1:B:52:ARG:HD3 | 2:C:657:TYR:HD1 | 1.69 | 0.57 |
| 2:BJ:1000:THR:HG22 | 2:BJ:1001:PHE:H | 1.70 | 0.57 |
| 2:BJ:77:THR:HG22 | 2:BJ:101:GLU:HB3 | 1.86 | 0.57 |
| 2:BJ:167:ILE:O | 2:BJ:168:ILE:HG22 | 2.05 | 0.57 |
| 3:CB:97:ASP:O | 3:CB:103:PRO:HB3 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CD:131:LYS:N | 4:CD:160:TRP:O | 2.29 | 0.57 |
| 5:CF:594:THR:OG1 | 5:CG:517:GLY:N | 2.37 | 0.57 |
| 5:CG:590:GLN:HE21 | 5:CH:486:VAL:HG11 | 1.69 | 0.57 |
| 5:CH:328:LEU:HG | 5:CH:329:PHE:H | 1.70 | 0.57 |
| 6:CJ:192:THR:HB | 6:CJ:219:ALA:HB3 | 1.87 | 0.57 |
| 7:DB:40:SER:HB3 | 7:DC:24:ASN:HB3 | 1.87 | 0.57 |
| 7:DC:386:ASN:HB2 | 7:DC:387:PRO:HD2 | 1.85 | 0.57 |
| 7:DD:466:SER:HB3 | 7:DD:468:PHE:CE2 | 2.40 | 0.57 |
| 7:DD:54:THR:HG22 | 7:DD:55:LYS:O | 2.05 | 0.57 |
| 11:DI:88:THR:H | 11:DI:163:ASN:HD21 | 1.53 | 0.57 |
| 1:EA:112:LEU:HB2 | 1:EA:300:ILE:HG22 | 1.86 | 0.57 |
| 2:EC:376:PHE:CB | 2:EC:405:VAL:HA | 2.35 | 0.57 |
| 2:EC:575:PHE:HB2 | 2:EC:608:VAL:HG22 | 1.85 | 0.57 |
| 3:ED:48:SER:OG | 3:ED:49:SER:N | 2.37 | 0.57 |
| 5:EJ:206:PHE:HZ | 5:EJ:221:GLU:HG2 | 1.70 | 0.57 |
| 5:EI:326:MET:HE3 | 5:EJ:279:SER:HB2 | 1.85 | 0.57 |
| 5:EJ:503:ASN:OD1 | 5:EJ:504:ASN:ND2 | 2.38 | 0.57 |
| 7:FE:440:GLN:OE1 | 7:FE:511:GLU:HG3 | 2.05 | 0.57 |
| 7:FF:118:PRO:HA | 7:FF:121:PHE:HB3 | 1.86 | 0.57 |
| 11:GB:40:LEU:HD21 | 11:GB:45:LEU:HD11 | 1.85 | 0.57 |
| 1:GE:594:GLU:N | 1:GE:594:GLU:OE1 | 2.38 | 0.57 |
| 2:GF:296:THR:OG1 | 2:GF:298:ALA:O | 2.23 | 0.57 |
| 2:GF:338:PHE:HE2 | 2:GF:342:SER:O | 1.87 | 0.57 |
| 2:GF:848:LEU:O | 2:GF:850:ASN:N | 2.37 | 0.57 |
| 3:GG:116:SER:HA | 3:GG:128:TRP:NE1 | 2.19 | 0.57 |
| 4:GI:141:SER:HB3 | 4:GI:164:ILE:HD11 | 1.87 | 0.57 |
| 4:GI:202:LEU:HA | 4:GI:278:VAL:HA | 1.87 | 0.57 |
| 5:HC:132:ASP:OD2 | 5:HC:151:ILE:N | 2.36 | 0.57 |
| 5:HC:503:ASN:OD1 | 5:HC:504:ASN:ND2 | 2.38 | 0.57 |
| 5:HD:328:LEU:HG | 5:HD:329:PHE:H | 1.70 | 0.57 |
| 5:HD:469:PRO:HA | 5:HD:472:TYR:CE2 | 2.39 | 0.57 |
| 8:IB:14:ASP:OD2 | 8:IB:17:ARG:NH2 | 2.33 | 0.57 |
| 9:IC:98:VAL:HB | 9:IC:103:THR:HB | 1.86 | 0.57 |
| 6:L:107:VAL:O | 6:L:114:VAL:N | 2.37 | 0.57 |
| 6:N:107:VAL:O | 6:N:114:VAL:N | 2.37 | 0.57 |
| 7:P:40:SER:O | 7:Q:24:ASN:ND2 | 2.36 | 0.57 |
| 7:Q:142:ILE:HG21 | 7:Q:157:THR:O | 2.04 | 0.57 |
| 7:Q:418:ASP:OD1 | 7:Q:422:LYS:N | 2.28 | 0.57 |
| 7:Q:54:THR:HG22 | 7:Q:55:LYS:O | 2.05 | 0.57 |
| 1:X:526:PRO:HB3 | 13:YA:254[D]:ARG:HD3 | 1.86 | 0.57 |
| 13:YA:76[B]:PRO:C | 13:YC:61[B]:ILE:HA | 2.25 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:575[C]:GLY:N | 13:YB:567[C]:ILE:O | 2.37 | 0.57 |
| 13:YC:50[F]:GLU:N | 13:YC:50[F]:GLU:OE2 | 2.33 | 0.57 |
| 13:YA:83[C]:TYR:CZ | 13:YC:95[C]:ILE:HD11 | 2.39 | 0.57 |
| 14:YD:35[C]:ILE:HD11 | 14:YD:38[C]:LEU:HB2 | 1.87 | 0.57 |
| 14:YD:35[E]:ILE:HD11 | 14:YD:38[E]:LEU:HB2 | 1.87 | 0.57 |
| 2:Z:125:GLU:HG2 | 2:Z:134:TYR:CD1 | 2.40 | 0.57 |
| 2:Z:522:THR:HG22 | 2:Z:536:TYR:HB3 | 1.86 | 0.57 |
| 2:Z:814:HIS:HB2 | 2:Z:862:TYR:HE1 | 1.69 | 0.57 |
| 1:A:338:ARG:NH2 | 1:B:340:VAL:O | 2.38 | 0.56 |
| 1:A:424:TYR:HA | 1:A:476:ILE:HG12 | 1.86 | 0.56 |
| 4:AA:131:LYS:N | 4:AA:160:TRP:O | 2.29 | 0.56 |
| 5:AC:255:ARG:CZ | 5:AE:390:LEU:HD12 | 2.35 | 0.56 |
| 5:AC:344:VAL:HG12 | 5:AC:349:TRP:H | 1.70 | 0.56 |
| 5:AC:358:VAL:HA | 5:AC:371:PHE:HA | 1.86 | 0.56 |
| 5:AE:168:LEU:HA | 5:AE:241:THR:HG22 | 1.87 | 0.56 |
| 7:AI:445:HIS:CE1 | 7:AJ:445:HIS:NE2 | 2.72 | 0.56 |
| 7:BA:192:GLN:O | 7:BA:208:TYR:HA | 2.05 | 0.56 |
| 7:BA:406:GLY:O | 7:BA:410:THR:HG23 | 2.05 | 0.56 |
| 8:BC:53:PHE:CD2 | 8:BC:54:MET:HG2 | 2.39 | 0.56 |
| 1:BI:184:PRO:HB2 | 1:BI:186:ILE:HD11 | 1.86 | 0.56 |
| 1:BI:148:ARG:NH2 | 1:BI:196:GLN:HE22 | 2.04 | 0.56 |
| 1:BI:452:VAL:O | 1:BI:457:SER:OG | 2.22 | 0.56 |
| 2:BJ:189:ARG:HG2 | 2:BJ:204:ARG:HH12 | 1.69 | 0.56 |
| 2:BJ:64:ASN:OD1 | 2:BJ:65:ASN:N | 2.33 | 0.56 |
| 2:BJ:741:GLU:OE2 | 2:BJ:745:LYS:NZ | 2.38 | 0.56 |
| 2:C:125:GLU:HG2 | 2:C:134:TYR:CD1 | 2.40 | 0.56 |
| 2:C:816:LEU:H | 3:E:201:ASN:ND2 | 2.02 | 0.56 |
| 2:C:963:TYR:CD1 | 2:C:964:PRO:HD2 | 2.39 | 0.56 |
| 5:CF:174:GLN:HE21 | 5:CF:177:PHE:HE1 | 1.53 | 0.56 |
| 5:CF:326:MET:CE | 5:CG:264:ARG:HB3 | 2.35 | 0.56 |
| 6:CI:12:SER:CB | 6:DA:6:ASN:HB3 | 2.35 | 0.56 |
| 7:DC:214:THR:HA | 7:DC:217:ASN:HD21 | 1.70 | 0.56 |
| 7:DD:406:GLY:O | 7:DD:410:THR:HG23 | 2.05 | 0.56 |
| 11:DI:186:ARG:CG | 11:DI:187:ILE:HG12 | 2.35 | 0.56 |
| 2:EC:167:ILE:O | 2:EC:168:ILE:HG22 | 2.05 | 0.56 |
| 2:EC:376:PHE:HB3 | 2:EC:405:VAL:HA | 1.86 | 0.56 |
| 2:EC:929:TYR:CD2 | 2:EC:961:VAL:HB | 2.39 | 0.56 |
| 4:EH:202:LEU:HA | 4:EH:278:VAL:HA | 1.87 | 0.56 |
| 6:FD:192:THR:HB | 6:FD:219:ALA:HB3 | 1.87 | 0.56 |
| 7:FE:199:VAL:HG12 | 7:FG:212:PRO:HG3 | 1.87 | 0.56 |
| 4:G:141:SER:HB3 | 4:G:164:ILE:HD11 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:GA:143:PHE:CE2 | 10:ID:349:ARG:HD3 | 2.40 | 0.56 |
| 12:DJ:144:ASN:H | 10:GA:58:TYR:HE1 | 1.53 | 0.56 |
| 11:GB:186:ARG:CG | 11:GB:187:ILE:HG12 | 2.35 | 0.56 |
| 12:GC:19:ASN:OD1 | 12:IF:228:LEU:HA | 2.05 | 0.56 |
| 12:GC:216:PHE:CE1 | 12:GC:218:MET:HE3 | 2.40 | 0.56 |
| 2:GF:340:PRO:HA | 2:GF:345:TYR:HE1 | 1.67 | 0.56 |
| 2:GF:814:HIS:HB2 | 2:GF:862:TYR:HE1 | 1.69 | 0.56 |
| 4:GI:166:SER:H | 4:HA:172:GLU:HA | 1.70 | 0.56 |
| 4:H:67:TYR:HD1 | 4:H:84:ARG:HB3 | 1.70 | 0.56 |
| 4:HA:67:TYR:HD1 | 4:HA:84:ARG:HB3 | 1.70 | 0.56 |
| 5:HB:358:VAL:HA | 5:HB:371:PHE:HA | 1.86 | 0.56 |
| 5:HB:43:PRO:HG2 | 5:HD:36:GLU:HG3 | 1.87 | 0.56 |
| 5:HC:213:GLY:O | 5:HC:214:SER:OG | 2.22 | 0.56 |
| 7:HI:44:VAL:HG21 | 7:HJ:25:PHE:HB3 | 1.87 | 0.56 |
| 9:IC:104:LEU:O | 9:IC:126:LEU:N | 2.31 | 0.56 |
| 5:I:326:MET:CE | 5:J:264:ARG:HB3 | 2.34 | 0.56 |
| 6:M:192:THR:HB | 6:M:219:ALA:HB3 | 1.87 | 0.56 |
| 7:P:447:HIS:HD2 | 7:Q:447:HIS:CD2 | 2.23 | 0.56 |
| 7:P:44:VAL:HG21 | 7:Q:25:PHE:HB3 | 1.86 | 0.56 |
| 7:O:301:ARG:HB3 | 7:Q:295:ILE:HG13 | 1.87 | 0.56 |
| 7:Q:406:GLY:O | 7:Q:410:THR:HG23 | 2.05 | 0.56 |
| 9:T:53:PHE:HA | 9:T:84:TYR:HE2 | 1.70 | 0.56 |
| 1:Y:111:MET:HB3 | 1:Y:164:ARG:HG2 | 1.86 | 0.56 |
| 13:YA:399[F]:HIS:CD2 | 13:YB:403[F]:PHE:HB3 | 2.39 | 0.56 |
| 13:YA:57[D]:VAL:CG1 | 13:YA:76[D]:PRO:HD3 | 2.34 | 0.56 |
| 13:YB:416[F]:HIS:HD2 | 13:YB:418[F]:THR:H | 1.51 | 0.56 |
| 13:YB:61[D]:ILE:HG21 | 13:YC:59[D]:GLN:CA | 2.24 | 0.56 |
| 13:YB:88[A]:ASP:N | 13:YB:88[A]:ASP:OD1 | 2.37 | 0.56 |
| 13:YC:17[C]:ASP:OD1 | 13:YC:19[C]:MET:N | 2.38 | 0.56 |
| 1:BH:526:PRO:HB3 | 13:YC:254[B]:ARG:HD3 | 1.87 | 0.56 |
| 13:YC:25[B]:GLY:HA3 | 13:YC:73[B]:VAL:HG12 | 1.87 | 0.56 |
| 13:YB:321[A]:LYS:HG2 | 13:YC:453[A]:ASP:OD1 | 2.05 | 0.56 |
| 13:YB:474[B]:ILE:HG12 | 13:YC:466[B]:ASN:HB2 | 1.86 | 0.56 |
| 13:YA:76[F]:PRO:C | 13:YC:61[F]:ILE:HA | 2.24 | 0.56 |
| 13:YA:90[C]:TRP:NE1 | 14:YD:175[C]:GLU:OE1 | 2.37 | 0.56 |
| 14:YE:35[E]:ILE:HD11 | 14:YE:38[E]:LEU:HB2 | 1.87 | 0.56 |
| 14:YE:64[E]:MET:HE3 | 14:YE:68[E]:GLU:HG3 | 1.87 | 0.56 |
| 2:Z:77:THR:HG22 | 2:Z:101:GLU:HB3 | 1.86 | 0.56 |
| 2:Z:146:LEU:HD13 | 2:Z:582:ALA:HB1 | 1.87 | 0.56 |
| 1:A:201:VAL:HG22 | 1:A:202:ASP:H | 1.70 | 0.56 |
| 1:A:558:PHE:O | 1:A:586:ARG:HB2 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:174:GLN:HE21 | 5:AC:177:PHE:HE1 | 1.54 | 0.56 |
| 6:AF:32:ARG:NH1 | 6:AG:144:ASN:OD1 | 2.35 | 0.56 |
| 6:AG:57:ASN:HB2 | 6:AH:164:GLN:NE2 | 2.20 | 0.56 |
| 7:AJ:394:ASP:OD2 | 7:BA:407:SER:N | 2.31 | 0.56 |
| 1:B:184:PRO:HB2 | 1:B:186:ILE:HD11 | 1.86 | 0.56 |
| 10:BE:39:PRO:HG3 | 10:BE:42:ARG:HH21 | 1.70 | 0.56 |
| 11:BF:88:THR:H | 11:BF:163:ASN:HD21 | 1.53 | 0.56 |
| 12:BG:216:PHE:HE1 | 12:BG:218:MET:HE3 | 1.70 | 0.56 |
| 2:C:338:PHE:HE2 | 2:C:342:SER:O | 1.87 | 0.56 |
| 2:C:775:ASP:O | 2:C:776:SER:OG | 2.20 | 0.56 |
| 2:C:773:GLN:N | 2:C:837:GLU:O | 2.33 | 0.56 |
| 2:C:929:TYR:CD2 | 2:C:961:VAL:HB | 2.39 | 0.56 |
| 3:CB:64:SER:HG | 3:CB:67:GLY:H | 1.51 | 0.56 |
| 4:CD:202:LEU:HB3 | 4:CD:278:VAL:HG22 | 1.87 | 0.56 |
| 4:CE:202:LEU:HA | 4:CE:278:VAL:HA | 1.87 | 0.56 |
| 5:CF:213:GLY:HA2 | 5:CF:221:GLU:HB2 | 1.87 | 0.56 |
| 5:CF:30:PHE:HE1 | 5:CH:30:PHE:CE1 | 2.24 | 0.56 |
| 5:CF:36:GLU:HA | 5:CF:50:LYS:NZ | 2.20 | 0.56 |
| 5:CF:60:LEU:HG | 5:CF:79:ILE:HG22 | 1.87 | 0.56 |
| 5:CG:73:SER:HB3 | 5:CG:101:THR:HG21 | 1.87 | 0.56 |
| 7:DB:399:PHE:HZ | 7:DB:516:ASN:HD22 | 1.53 | 0.56 |
| 7:DB:212:PRO:HG3 | 7:DC:199:VAL:HG12 | 1.87 | 0.56 |
| 1:EA:494:THR:HG21 | 1:EA:603:TYR:HA | 1.86 | 0.56 |
| 1:EB:102:SER:H | 1:EB:194:ARG:NH1 | 2.02 | 0.56 |
| 2:EC:19:ASN:OD1 | 2:EC:20:GLN:HG3 | 2.05 | 0.56 |
| 2:EC:435:SER:HB3 | 2:EC:512:PRO:HA | 1.86 | 0.56 |
| 4:EH:239:ARG:HD2 | 4:EH:249:ILE:HD12 | 1.85 | 0.56 |
| 5:EI:195:HIS:HE2 | 5:EI:236:CYS:HG | 1.53 | 0.56 |
| 5:EI:71:ASN:OD1 | 5:EI:73:SER:N | 2.27 | 0.56 |
| 4:F:282:GLN:NE2 | 4:H:275:ALA:O | 2.37 | 0.56 |
| 5:FA:328:LEU:HG | 5:FA:329:PHE:H | 1.70 | 0.56 |
| 7:FF:418:ASP:OD1 | 7:FF:422:LYS:N | 2.38 | 0.56 |
| 7:FG:54:THR:HG22 | 7:FG:55:LYS:O | 2.05 | 0.56 |
| 8:FH:14:ASP:HB2 | 8:IB:104:PRO:HD3 | 1.88 | 0.56 |
| 8:FH:53:PHE:CD2 | 8:FH:54:MET:HG2 | 2.39 | 0.56 |
| 2:GF:376:PHE:HB3 | 2:GF:405:VAL:HA | 1.86 | 0.56 |
| 2:GF:724:ALA:O | 2:GF:726:PHE:N | 2.36 | 0.56 |
| 2:EC:581:TYR:OH | 2:GF:850:ASN:HB3 | 2.04 | 0.56 |
| 3:GH:29:GLY:HA3 | 3:GH:34:LYS:HB2 | 1.88 | 0.56 |
| 5:HC:290:SER:CB | 5:HC:370:HIS:HA | 2.35 | 0.56 |
| 5:HD:299:ILE:O | 5:HD:301:GLY:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HF:192:THR:HB | 6:HF:219:ALA:HB3 | 1.87 | 0.56 |
| 7:HJ:192:GLN:O | 7:HJ:208:TYR:HA | 2.05 | 0.56 |
| 7:HJ:406:GLY:O | 7:HJ:410:THR:HG23 | 2.05 | 0.56 |
| 5:K:328:LEU:HG | 5:K:329:PHE:H | 1.70 | 0.56 |
| 7:Q:9:VAL:HG23 | 7:Q:10:SER:N | 2.20 | 0.56 |
| 11:V:88:THR:H | 11:V:163:ASN:HD21 | 1.53 | 0.56 |
| 1:X:112:LEU:HB2 | 1:X:300:ILE:HG22 | 1.86 | 0.56 |
| 1:X:147:SER:HA | 1:X:167:LEU:HD23 | 1.88 | 0.56 |
| 1:X:363:PHE:CG | 1:X:636:ASP:HB2 | 2.39 | 0.56 |
| 1:Y:229:THR:OG1 | 1:Y:233:ASN:O | 2.23 | 0.56 |
| 1:X:400:ASN:H | 1:Y:341:THR:HG22 | 1.69 | 0.56 |
| 1:Y:70:PHE:HE2 | 2:Z:686:LEU:CB | 2.18 | 0.56 |
| 1:Y:76:TYR:HB3 | 1:Y:82:THR:HG21 | 1.87 | 0.56 |
| 13:YA:376[F]:PHE:CE2 | 13:YB:447[F]:ASN:HB3 | 2.40 | 0.56 |
| 13:YA:527[A]:THR:O | 13:YB:519[A]:THR:HA | 2.05 | 0.56 |
| 13:YA:88[C]:ASP:N | 13:YA:88[C]:ASP:OD1 | 2.38 | 0.56 |
| 13:YA:88[D]:ASP:OD1 | 13:YA:88[D]:ASP:N | 2.38 | 0.56 |
| 13:YB:169[B]:ASP:HB2 | 13:YB:343[B]:VAL:HB | 1.86 | 0.56 |
| 13:YA:399[A]:HIS:CD2 | 13:YB:403[A]:PHE:HB3 | 2.39 | 0.56 |
| 14:YD:125[B]:PHE:CE2 | 14:YD:134[B]:GLU:HG3 | 2.30 | 0.56 |
| 13:YA:90[F]:TRP:NE1 | 14:YD:175[F]:GLU:OE1 | 2.35 | 0.56 |
| 14:YD:349[E]:ASN:OD1 | 14:YD:350[E]:ASN:N | 2.38 | 0.56 |
| 14:YD:35[B]:ILE:HD11 | 14:YD:38[B]:LEU:HB2 | 1.87 | 0.56 |
| 14:YD:64[B]:MET:HE3 | 14:YD:68[B]:GLU:HG3 | 1.87 | 0.56 |
| 14:YF:35[E]:ILE:HD11 | 14:YF:38[E]:LEU:HB2 | 1.87 | 0.56 |
| 14:YF:64[C]:MET:HE3 | 14:YF:68[C]:GLU:HG3 | 1.87 | 0.56 |
| 2:Z:338:PHE:HE2 | 2:Z:342:SER:O | 1.87 | 0.56 |
| 1:X:5:PRO:HG2 | 2:Z:674:TYR:HA | 1.87 | 0.56 |
| 2:Z:800:ARG:HB3 | 2:Z:809:TRP:CZ3 | 2.40 | 0.56 |
| 5:AD:290:SER:CB | 5:AD:370:HIS:HA | 2.35 | 0.56 |
| 5:AD:600:ARG:NE | 5:AD:602:ALA:O | 2.32 | 0.56 |
| 7:AI:12:GLU:HB3 | 7:AI:15:TYR:HB3 | 1.86 | 0.56 |
| 7:AI:514:PRO:HG2 | 7:AJ:399:PHE:CD2 | 2.40 | 0.56 |
| 7:AI:40:SER:HB3 | 7:AJ:24:ASN:HB3 | 1.87 | 0.56 |
| 1:BH:147:SER:HA | 1:BH:167:LEU:HD23 | 1.88 | 0.56 |
| 1:BI:363:PHE:CD1 | 1:BI:636:ASP:HB2 | 2.39 | 0.56 |
| 2:BJ:712:ASN:HD21 | 2:BJ:720:ARG:HG3 | 1.70 | 0.56 |
| 2:C:522:THR:HG22 | 2:C:536:TYR:HB3 | 1.86 | 0.56 |
| 2:C:675:LEU:O | 2:C:681:THR:HB | 2.04 | 0.56 |
| 2:C:814:HIS:HB2 | 2:C:862:TYR:HE1 | 1.69 | 0.56 |
| 2:C:98:GLU:OE1 | 2:C:98:GLU:N | 2.30 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:CA:117:ALA:H | 3:CA:120:ASN:HB3 | 1.70 | 0.56 |
| 3:CA:116:SER:HA | 3:CA:128:TRP:NE1 | 2.20 | 0.56 |
| 5:CF:252:SER:OG | 5:CF:393:LEU:HB3 | 2.06 | 0.56 |
| 5:CH:168:LEU:HA | 5:CH:241:THR:HG22 | 1.87 | 0.56 |
| 5:CH:562:SER:C | 5:CH:564:PRO:HD3 | 2.26 | 0.56 |
| 6:CI:15:ALA:HB2 | 6:DA:52:ILE:HD11 | 1.87 | 0.56 |
| 3:D:114:CYS:HA | 3:D:120:ASN:OD1 | 2.05 | 0.56 |
| 7:DC:192:GLN:NE2 | 7:DD:185:GLU:O | 2.33 | 0.56 |
| 8:DF:10:PHE:C | 8:DF:12:SER:H | 2.08 | 0.56 |
| 9:DG:98:VAL:HB | 9:DG:103:THR:HB | 1.86 | 0.56 |
| 2:EC:1000:THR:HG22 | 2:EC:1001:PHE:H | 1.70 | 0.56 |
| 2:EC:1012:LEU:HD13 | 2:EC:1027:GLN:OE1 | 2.05 | 0.56 |
| 2:EC:125:GLU:HG2 | 2:EC:134:TYR:CD1 | 2.40 | 0.56 |
| 2:EC:420:THR:O | 2:EC:424:ARG:NE | 2.38 | 0.56 |
| 3:ED:117:ALA:H | 3:ED:120:ASN:HB3 | 1.70 | 0.56 |
| 4:EF:202:LEU:HA | 4:EF:278:VAL:HA | 1.87 | 0.56 |
| 4:F:67:TYR:HD1 | 4:F:84:ARG:HB3 | 1.70 | 0.56 |
| 7:FE:399:PHE:HZ | 7:FE:516:ASN:HD22 | 1.53 | 0.56 |
| 7:FF:214:THR:HA | 7:FF:217:ASN:HD21 | 1.70 | 0.56 |
| 7:FG:9:VAL:HG23 | 7:FG:10:SER:N | 2.20 | 0.56 |
| 8:FH:10:PHE:C | 8:FH:12:SER:H | 2.08 | 0.56 |
| 8:FI:53:PHE:CD2 | 8:FI:54:MET:HG2 | 2.39 | 0.56 |
| 4:G:67:TYR:HD1 | 4:G:84:ARG:HB3 | 1.70 | 0.56 |
| 1:GD:87:SER:OG | 1:GD:230:ILE:O | 2.21 | 0.56 |
| 1:GD:363:PHE:CG | 1:GD:636:ASP:HB2 | 2.40 | 0.56 |
| 2:GF:1012:LEU:HD13 | 2:GF:1027:GLN:OE1 | 2.05 | 0.56 |
| 4:GI:202:LEU:HB3 | 4:GI:278:VAL:HG22 | 1.86 | 0.56 |
| 4:H:131:LYS:N | 4:H:160:TRP:O | 2.29 | 0.56 |
| 5:HB:344:VAL:HG12 | 5:HB:349:TRP:H | 1.70 | 0.56 |
| 7:HH:514:PRO:HG2 | 7:HI:399:PHE:CD2 | 2.40 | 0.56 |
| 7:HI:394:ASP:OD2 | 7:HJ:407:SER:N | 2.31 | 0.56 |
| 5:I:174:GLN:HE21 | 5:I:177:PHE:HE1 | 1.53 | 0.56 |
| 5:I:344:VAL:HG12 | 5:I:349:TRP:H | 1.70 | 0.56 |
| 7:O:497:ASN:H | 7:O:500:TYR:HB2 | 1.71 | 0.56 |
| 7:O:440:GLN:OE1 | 7:O:511:GLU:HG3 | 2.05 | 0.56 |
| 7:P:118:PRO:HA | 7:P:121:PHE:HB3 | 1.86 | 0.56 |
| 13:YA:61[C]:ILE:HD11 | 13:YB:72[C]:SER:O | 2.05 | 0.56 |
| 13:YB:88[B]:ASP:OD1 | 13:YB:88[B]:ASP:N | 2.38 | 0.56 |
| 13:YB:321[E]:LYS:HG2 | 13:YC:453[E]:ASP:OD1 | 2.05 | 0.56 |
| 13:YC:58[B]:ILE:HG12 | 13:YC:97[B]:LEU:HD22 | 1.88 | 0.56 |
| 13:YC:82[E]:VAL:HG22 | 13:YC:98[E]:GLY:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:64[F]:MET:HE3 | 14:YD:68[F]:GLU:HG3 | 1.87 | 0.56 |
| 14:YE:125[F]:PHE:CE2 | 14:YE:134[F]:GLU:HG3 | 2.30 | 0.56 |
| 14:YF:125[D]:PHE:CE2 | 14:YF:134[D]:GLU:HG3 | 2.30 | 0.56 |
| 14:YF:35[F]:ILE:HD11 | 14:YF:38[F]:LEU:HB2 | 1.88 | 0.56 |
| 14:YF:64[B]:MET:HE3 | 14:YF:68[B]:GLU:HG3 | 1.87 | 0.56 |
| 14:YF:98[D]:ASP:OD1 | 14:YF:99[D]:SER:N | 2.39 | 0.56 |
| 2:Z:741:GLU:OE2 | 2:Z:745:LYS:NZ | 2.38 | 0.56 |
| 4:AB:202:LEU:HA | 4:AB:278:VAL:HA | 1.87 | 0.56 |
| 5:AD:419:ASP:HB3 | 5:AD:436:VAL:HB | 1.86 | 0.56 |
| 5:AD:49:TRP:HZ3 | 5:AD:96:ARG:HD2 | 1.70 | 0.56 |
| 5:AE:299:ILE:O | 5:AE:301:GLY:N | 2.38 | 0.56 |
| 5:AE:328:LEU:HG | 5:AE:329:PHE:H | 1.70 | 0.56 |
| 11:BF:57:GLU:N | 11:BF:57:GLU:OE1 | 2.25 | 0.56 |
| 12:BG:126:TYR:HA | 12:DJ:230:TYR:CD2 | 2.40 | 0.56 |
| 12:BG:177:TRP:CZ3 | 12:BG:220:SER:HB3 | 2.38 | 0.56 |
| 12:BG:22:PHE:HA | 12:BG:203:LEU:HA | 1.86 | 0.56 |
| 1:BI:90:VAL:HG13 | 1:BI:100:PRO:HG3 | 1.87 | 0.56 |
| 2:BJ:808:GLN:NE2 | 2:BJ:839:ILE:HG13 | 2.21 | 0.56 |
| 3:CA:261:ALA:O | 3:CA:266:ASN:ND2 | 2.30 | 0.56 |
| 3:CB:96:GLY:HA2 | 3:CB:104:TYR:CE1 | 2.41 | 0.56 |
| 5:CG:503:ASN:OD1 | 5:CG:504:ASN:ND2 | 2.38 | 0.56 |
| 5:CH:217:GLU:HB2 | 5:CH:222:LEU:HB2 | 1.88 | 0.56 |
| 7:DB:514:PRO:HB3 | 7:DC:512:THR:O | 2.05 | 0.56 |
| 7:DC:12:GLU:HG3 | 7:DC:15:TYR:H | 1.71 | 0.56 |
| 5:CG:200:LEU:HD22 | 7:DC:2:SER:HA | 1.88 | 0.56 |
| 7:DC:466:SER:HB3 | 7:DC:468:PHE:HE2 | 1.71 | 0.56 |
| 8:DE:10:PHE:C | 8:DE:12:SER:H | 2.08 | 0.56 |
| 1:EA:399:TYR:O | 1:EA:400:ASN:HB2 | 2.04 | 0.56 |
| 1:EB:229:THR:OG1 | 1:EB:233:ASN:O | 2.23 | 0.56 |
| 1:EA:338:ARG:NH2 | 1:EB:340:VAL:O | 2.37 | 0.56 |
| 1:EB:363:PHE:CD1 | 1:EB:636:ASP:HB2 | 2.39 | 0.56 |
| 1:EB:52:ARG:HD3 | 2:EC:657:TYR:HD1 | 1.69 | 0.56 |
| 2:EC:10:SER:HB3 | 2:EC:26:ASP:HB2 | 1.88 | 0.56 |
| 2:EC:741:GLU:OE2 | 2:EC:745:LYS:NZ | 2.38 | 0.56 |
| 3:ED:135:ASP:OD1 | 3:ED:136:VAL:N | 2.35 | 0.56 |
| 4:EG:171:LYS:HB2 | 4:EH:165:GLU:HB3 | 1.88 | 0.56 |
| 5:EI:174:GLN:HE21 | 5:EI:177:PHE:HE1 | 1.53 | 0.56 |
| 5:EI:214:SER:OG | 5:EI:222:LEU:O | 2.22 | 0.56 |
| 5:EI:344:VAL:HG12 | 5:EI:349:TRP:H | 1.70 | 0.56 |
| 5:EI:36:GLU:HA | 5:EI:50:LYS:NZ | 2.20 | 0.56 |
| 5:EJ:213:GLY:O | 5:EJ:214:SER:OG | 2.22 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:992:PRO:HB3 | 5:FA:19:LEU:HB3 | 1.87 | 0.56 |
| 5:FA:237:ASN:OD1 | 5:FA:238:ILE:N | 2.38 | 0.56 |
| 7:Q:476:ASP:HB2 | 5:FA:353:HIS:NE2 | 2.19 | 0.56 |
| 5:FA:357:SER:OG | 6:FC:4:LEU:HD21 | 2.06 | 0.56 |
| 6:FB:12:SER:CB | 6:FD:6:ASN:HB3 | 2.36 | 0.56 |
| 6:FC:69:THR:HA | 6:FD:73:ASN:HB3 | 1.88 | 0.56 |
| 7:FE:263:VAL:O | 7:FF:255:SER:OG | 2.13 | 0.56 |
| 7:FF:310:ASN:OD1 | 7:FF:311:GLY:N | 2.39 | 0.56 |
| 7:FE:514:PRO:HG2 | 7:FF:399:PHE:CD2 | 2.40 | 0.56 |
| 8:R:96:GLY:O | 8:FH:56:ARG:NH2 | 2.38 | 0.56 |
| 2:GF:555:ARG:HG3 | 2:GF:557:VAL:H | 1.68 | 0.56 |
| 2:GF:741:GLU:OE2 | 2:GF:745:LYS:NZ | 2.38 | 0.56 |
| 2:GF:800:ARG:HB3 | 2:GF:809:TRP:CZ3 | 2.40 | 0.56 |
| 3:GG:117:ALA:H | 3:GG:120:ASN:HB3 | 1.70 | 0.56 |
| 3:GH:195:PRO:HD3 | 3:GH:223:TRP:HD1 | 1.65 | 0.56 |
| 5:HB:174:GLN:HE21 | 5:HB:177:PHE:HE1 | 1.53 | 0.56 |
| 5:HB:252:SER:OG | 5:HB:393:LEU:HB3 | 2.06 | 0.56 |
| 5:HC:392:THR:OG1 | 5:HD:305:ASN:ND2 | 2.38 | 0.56 |
| 5:HC:73:SER:HB3 | 5:HC:101:THR:HG21 | 1.87 | 0.56 |
| 7:HI:466:SER:HB3 | 7:HI:468:PHE:HE2 | 1.71 | 0.56 |
| 7:HJ:466:SER:HB3 | 7:HJ:468:PHE:CE2 | 2.40 | 0.56 |
| 5:I:195:HIS:HE2 | 5:I:236:CYS:HG | 1.53 | 0.56 |
| 5:I:36:GLU:HG3 | 5:J:43:PRO:HG2 | 1.86 | 0.56 |
| 5:J:600:ARG:NE | 5:J:602:ALA:O | 2.32 | 0.56 |
| 7:O:12:GLU:HB3 | 7:O:15:TYR:HB3 | 1.86 | 0.56 |
| 7:O:513:ARG:O | 7:P:441:GLN:N | 2.30 | 0.56 |
| 7:Q:49:ASP:HA | 7:Q:57:ILE:O | 2.05 | 0.56 |
| 2:C:654:PRO:HG3 | 9:T:47:ARG:HD2 | 1.86 | 0.56 |
| 10:U:349:ARG:HD3 | 10:ID:143:PHE:CE2 | 2.41 | 0.56 |
| 12:W:247:VAL:HG12 | 12:W:248:MET:H | 1.71 | 0.56 |
| 1:Y:346:ASP:HB2 | 1:Y:360:VAL:HG13 | 1.87 | 0.56 |
| 1:Y:400:ASN:OD1 | 1:Y:401:LEU:N | 2.39 | 0.56 |
| 1:Y:460:ALA:HA | 1:Y:631:VAL:HG12 | 1.87 | 0.56 |
| 13:YA:25[F]:GLY:HA3 | 13:YA:73[F]:VAL:HG12 | 1.87 | 0.56 |
| 13:YA:265[C]:VAL:HG22 | 13:YA:300[C]:LEU:HD23 | 1.88 | 0.56 |
| 13:YA:376[A]:PHE:CE2 | 13:YB:447[A]:ASN:HB3 | 2.40 | 0.56 |
| 13:YA:522[C]:VAL:HA | 13:YB:514[C]:VAL:O | 2.05 | 0.56 |
| 13:YA:89[E]:LYS:O | 13:YA:91[E]:LYS:HG3 | 2.06 | 0.56 |
| 13:YA:522[D]:VAL:HA | 13:YB:514[D]:VAL:O | 2.05 | 0.56 |
| 13:YB:284[F]:MET:HE3 | 13:YC:363[F]:PRO:CB | 2.36 | 0.56 |
| 14:YD:35[A]:ILE:HD11 | 14:YD:38[A]:LEU:HB2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:35[F]:ILE:HD11 | 14:YE:38[F]:LEU:HB2 | 1.88 | 0.56 |
| 14:YF:35[A]:ILE:HD11 | 14:YF:38[A]:LEU:HB2 | 1.88 | 0.56 |
| 14:YF:64[D]:MET:HE3 | 14:YF:68[D]:GLU:HG3 | 1.87 | 0.56 |
| 14:YF:98[A]:ASP:OD1 | 14:YF:99[A]:SER:N | 2.38 | 0.56 |
| 4:AA:202:LEU:HA | 4:AA:278:VAL:HA | 1.87 | 0.56 |
| 4:AB:67:TYR:HD1 | 4:AB:84:ARG:HB3 | 1.70 | 0.56 |
| 5:AC:569:TYR:CD1 | 5:AD:544:VAL:HA | 2.39 | 0.56 |
| 6:AH:192:THR:HB | 6:AH:219:ALA:HB3 | 1.87 | 0.56 |
| 7:AJ:214:THR:HA | 7:AJ:217:ASN:HD21 | 1.71 | 0.56 |
| 1:B:346:ASP:HB2 | 1:B:360:VAL:HG13 | 1.87 | 0.56 |
| 1:BH:555:ILE:O | 1:BH:589:TYR:HD1 | 1.87 | 0.56 |
| 1:BI:229:THR:OG1 | 1:BI:233:ASN:O | 2.23 | 0.56 |
| 1:BI:460:ALA:HA | 1:BI:631:VAL:HG12 | 1.87 | 0.56 |
| 2:BJ:420:THR:O | 2:BJ:424:ARG:NE | 2.38 | 0.56 |
| 2:C:1000:THR:HG22 | 2:C:1001:PHE:H | 1.70 | 0.56 |
| 4:CC:202:LEU:HB3 | 4:CC:278:VAL:HG22 | 1.87 | 0.56 |
| 5:CF:344:VAL:HG12 | 5:CF:349:TRP:H | 1.70 | 0.56 |
| 7:DC:418:ASP:OD1 | 7:DC:422:LYS:N | 2.38 | 0.56 |
| 7:DD:192:GLN:O | 7:DD:208:TYR:HA | 2.05 | 0.56 |
| 7:DD:418:ASP:OD1 | 7:DD:422:LYS:N | 2.28 | 0.56 |
| 7:DB:449:GLY:N | 7:DD:482:TYR:O | 2.31 | 0.56 |
| 10:DH:333:ALA:HA | 12:DJ:188:LEU:HD23 | 1.88 | 0.56 |
| 2:EC:77:THR:HG22 | 2:EC:101:GLU:HB3 | 1.86 | 0.56 |
| 3:ED:114:CYS:HA | 3:ED:120:ASN:OD1 | 2.05 | 0.56 |
| 5:FA:285:LEU:CD1 | 5:FA:375:PHE:HB2 | 2.36 | 0.56 |
| 5:FA:562:SER:C | 5:FA:564:PRO:HD3 | 2.26 | 0.56 |
| 7:FF:211:SER:N | 7:FF:214:THR:OG1 | 2.28 | 0.56 |
| 7:FF:466:SER:HB3 | 7:FF:468:PHE:HE2 | 1.71 | 0.56 |
| 7:FG:89:ASN:OD1 | 7:FG:90:ALA:N | 2.39 | 0.56 |
| 1:GD:212:LYS:HA | 1:GD:399:TYR:OH | 2.05 | 0.56 |
| 1:GE:111:MET:HB3 | 1:GE:164:ARG:HG2 | 1.86 | 0.56 |
| 1:GE:386:THR:O | 1:GE:389:ARG:N | 2.39 | 0.56 |
| 1:GE:90:VAL:HG13 | 1:GE:100:PRO:HG3 | 1.88 | 0.56 |
| 2:GF:211:VAL:N | 2:GF:220:LYS:O | 2.27 | 0.56 |
| 2:GF:77:THR:HG22 | 2:GF:101:GLU:HB3 | 1.87 | 0.56 |
| 3:GG:204:THR:HG21 | 3:GG:248:ARG:HH22 | 1.69 | 0.56 |
| 3:GH:104:TYR:HB3 | 3:GH:165:ARG:HB2 | 1.87 | 0.56 |
| 4:HA:141:SER:HB3 | 4:HA:164:ILE:HD11 | 1.87 | 0.56 |
| 5:HD:285:LEU:CD1 | 5:HD:375:PHE:HB2 | 2.36 | 0.56 |
| 7:HI:118:PRO:HA | 7:HI:121:PHE:HB3 | 1.86 | 0.56 |
| 5:I:326:MET:HE3 | 5:J:279:SER:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:199:VAL:HG12 | 7:Q:212:PRO:HG3 | 1.86 | 0.56 |
| 7:P:310:ASN:OD1 | 7:P:311:GLY:N | 2.39 | 0.56 |
| 7:Q:466:SER:HB3 | 7:Q:468:PHE:CE2 | 2.40 | 0.56 |
| 1:X:400:ASN:OD1 | 1:X:401:LEU:N | 2.38 | 0.56 |
| 1:Y:386:THR:O | 1:Y:389:ARG:N | 2.39 | 0.56 |
| 13:YA:376[D]:PHE:CE2 | 13:YB:447[D]:ASN:HB3 | 2.40 | 0.56 |
| 13:YA:82[B]:VAL:HG22 | 13:YA:98[B]:GLY:O | 2.05 | 0.56 |
| 13:YB:265[A]:VAL:HG22 | 13:YB:300[A]:LEU:HD23 | 1.88 | 0.56 |
| 13:YB:26[E]:ARG:HA | 13:YB:55[E]:MET:O | 2.05 | 0.56 |
| 13:YB:474[A]:ILE:HG12 | 13:YC:466[A]:ASN:HB2 | 1.86 | 0.56 |
| 13:YB:87[E]:LEU:HD21 | 13:YB:95[E]:ILE:HG23 | 1.87 | 0.56 |
| 13:YB:89[C]:LYS:O | 13:YB:91[C]:LYS:HG3 | 2.06 | 0.56 |
| 13:YC:88[F]:ASP:N | 13:YC:88[F]:ASP:OD1 | 2.38 | 0.56 |
| 13:YC:89[A]:LYS:O | 13:YC:91[A]:LYS:HG3 | 2.06 | 0.56 |
| 14:YD:35[F]:ILE:HD11 | 14:YD:38[F]:LEU:HB2 | 1.87 | 0.56 |
| 14:YD:50[F]:GLY:O | 14:YD:109[F]:LEU:N | 2.38 | 0.56 |
| 14:YE:50[D]:GLY:O | 14:YE:109[D]:LEU:N | 2.38 | 0.56 |
| 14:YE:64[A]:MET:HE3 | 14:YE:68[A]:GLU:HG3 | 1.87 | 0.56 |
| 14:YF:301[B]:MET:HA | 14:YF:304[B]:TYR:HD2 | 1.71 | 0.56 |
| 14:YF:35[B]:ILE:HD11 | 14:YF:38[B]:LEU:HB2 | 1.87 | 0.56 |
| 2:Z:161:SER:O | 2:Z:164:SER:N | 2.39 | 0.56 |
| 2:Z:376:PHE:CB | 2:Z:405:VAL:HA | 2.35 | 0.56 |
| 5:AC:146:VAL:HG23 | 5:AD:153:LYS:HB2 | 1.86 | 0.56 |
| 5:AC:409:SER:N | 5:AE:444:ASN:O | 2.32 | 0.56 |
| 6:AG:107:VAL:O | 6:AG:114:VAL:N | 2.37 | 0.56 |
| 7:AI:339:ARG:CZ | 7:BA:358:ALA:HB2 | 2.36 | 0.56 |
| 7:AJ:118:PRO:HA | 7:AJ:121:PHE:HB3 | 1.86 | 0.56 |
| 1:B:111:MET:HB3 | 1:B:164:ARG:HG2 | 1.87 | 0.56 |
| 10:BE:237:THR:HA | 10:BE:287:VAL:HG23 | 1.87 | 0.56 |
| 11:BF:142:LYS:HB3 | 11:BF:143:TYR:HD2 | 1.71 | 0.56 |
| 1:BH:209:TRP:HD1 | 1:BH:225:TYR:HE1 | 1.51 | 0.56 |
| 1:BI:582:ASN:HD21 | 1:BI:586:ARG:NH2 | 1.98 | 0.56 |
| 2:BJ:182:GLN:O | 2:BJ:210:LYS:NZ | 2.33 | 0.56 |
| 2:BJ:36:VAL:HG23 | 2:BJ:59:LEU:HB2 | 1.88 | 0.56 |
| 2:C:143:MET:HG2 | 2:C:544:VAL:HG22 | 1.87 | 0.56 |
| 2:C:458:ASP:OD1 | 2:C:472:LYS:HB2 | 2.06 | 0.56 |
| 2:C:800:ARG:HB3 | 2:C:809:TRP:CZ3 | 2.40 | 0.56 |
| 3:CB:170:PRO:HB3 | 3:CB:188:TRP:CG | 2.40 | 0.56 |
| 4:CE:67:TYR:HD1 | 4:CE:84:ARG:HB3 | 1.70 | 0.56 |
| 5:CH:299:ILE:O | 5:CH:301:GLY:N | 2.38 | 0.56 |
| 5:CF:255:ARG:CZ | 5:CH:390:LEU:HD12 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:204:THR:HG21 | 3:D:248:ARG:HH22 | 1.69 | 0.56 |
| 7:DB:406:GLY:O | 7:DB:410:THR:HG23 | 2.06 | 0.56 |
| 7:DB:514:PRO:HG2 | 7:DC:399:PHE:CD2 | 2.41 | 0.56 |
| 3:E:104:TYR:HB3 | 3:E:165:ARG:HB2 | 1.87 | 0.56 |
| 3:E:29:GLY:HA3 | 3:E:34:LYS:HB2 | 1.88 | 0.56 |
| 1:EB:148:ARG:NH2 | 1:EB:196:GLN:HE22 | 2.04 | 0.56 |
| 1:EB:209:TRP:HE3 | 1:EB:212:LYS:HB2 | 1.69 | 0.56 |
| 1:EB:452:VAL:O | 1:EB:457:SER:OG | 2.22 | 0.56 |
| 2:EC:793:CYS:HB3 | 2:EC:813:ILE:HG12 | 1.87 | 0.56 |
| 2:EC:800:ARG:HB3 | 2:EC:809:TRP:CZ3 | 2.40 | 0.56 |
| 2:BJ:506:MET:HB3 | 3:EE:176:ALA:HB1 | 1.87 | 0.56 |
| 5:EJ:290:SER:HA | 5:EJ:371:PHE:HB3 | 1.88 | 0.56 |
| 7:DC:71:ASN:CB | 7:FG:365:GLY:HA2 | 2.35 | 0.56 |
| 10:GA:333:ALA:HA | 12:GC:188:LEU:HD23 | 1.88 | 0.56 |
| 12:GC:218:MET:SD | 12:GC:243:PHE:CD2 | 2.99 | 0.56 |
| 1:GD:582:ASN:OD1 | 1:GD:585:GLY:N | 2.27 | 0.56 |
| 1:GE:102:SER:H | 1:GE:194:ARG:NH1 | 2.02 | 0.56 |
| 2:GF:20:GLN:HA | 2:GF:70:ASP:HA | 1.87 | 0.56 |
| 4:GJ:141:SER:HB3 | 4:GJ:164:ILE:HD11 | 1.87 | 0.56 |
| 4:F:7:LYS:HD3 | 4:H:39:TYR:CG | 2.41 | 0.56 |
| 5:HB:326:MET:HE3 | 5:HC:279:SER:HB2 | 1.87 | 0.56 |
| 5:HB:241:THR:HG21 | 5:HD:200:LEU:CD1 | 2.34 | 0.56 |
| 5:HD:217:GLU:HB2 | 5:HD:222:LEU:HB2 | 1.88 | 0.56 |
| 7:HH:14:ARG:NH2 | 7:HI:19:ASP:OD2 | 2.38 | 0.56 |
| 7:HH:339:ARG:CZ | 7:HJ:358:ALA:HB2 | 2.36 | 0.56 |
| 7:HH:399:PHE:HZ | 7:HH:516:ASN:HD22 | 1.53 | 0.56 |
| 7:HJ:89:ASN:OD1 | 7:HJ:90:ALA:N | 2.39 | 0.56 |
| 5:I:339:GLU:HB3 | 6:M:172:SER:O | 2.05 | 0.56 |
| 5:I:358:VAL:HA | 5:I:371:PHE:HA | 1.86 | 0.56 |
| 5:K:168:LEU:HA | 5:K:241:THR:HG22 | 1.87 | 0.56 |
| 13:YA:25[D]:GLY:HA3 | 13:YA:73[D]:VAL:HG12 | 1.86 | 0.56 |
| 13:YA:169[E]:ASP:HB2 | 13:YA:343[E]:VAL:HB | 1.86 | 0.56 |
| 13:YA:89[F]:LYS:O | 13:YA:91[F]:LYS:HG3 | 2.06 | 0.56 |
| 13:YB:265[B]:VAL:HG22 | 13:YB:300[B]:LEU:HD23 | 1.88 | 0.56 |
| 13:YB:474[F]:ILE:HG12 | 13:YC:466[F]:ASN:HB2 | 1.86 | 0.56 |
| 1:GD:526:PRO:HB3 | 13:YC:254[D]:ARG:HD3 | 1.86 | 0.56 |
| 13:YC:265[E]:VAL:HG22 | 13:YC:300[E]:LEU:HD23 | 1.88 | 0.56 |
| 13:YC:25[F]:GLY:HA3 | 13:YC:73[F]:VAL:HG12 | 1.87 | 0.56 |
| 13:YC:87[F]:LEU:HD21 | 13:YC:95[F]:ILE:HG23 | 1.86 | 0.56 |
| 13:YC:89[B]:LYS:O | 13:YC:91[B]:LYS:HG3 | 2.05 | 0.56 |
| 14:YD:98[B]:ASP:OD1 | 14:YD:99[B]:SER:N | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:98[E]:ASP:OD1 | 14:YD:99[E]:SER:N | 2.38 | 0.56 |
| 14:YE:189[C]:TRP:NE1 | 14:YE:320[C]:PRO:HG2 | 2.21 | 0.56 |
| 14:YE:301[C]:MET:HA | 14:YE:304[C]:TYR:HD2 | 1.71 | 0.56 |
| 11:GB:190:LYS:HE3 | 14:YF:24[B]:SER:O | 2.04 | 0.56 |
| 14:YF:292[D]:TYR:CD1 | 14:YF:371[D]:LYS:HB3 | 2.41 | 0.56 |
| 14:YF:98[C]:ASP:OD1 | 14:YF:99[C]:SER:N | 2.39 | 0.56 |
| 2:Z:319:TYR:HD1 | 2:Z:328:TYR:HB2 | 1.71 | 0.56 |
| 2:Z:808:GLN:NE2 | 2:Z:839:ILE:HG13 | 2.21 | 0.56 |
| 1:A:400:ASN:H | 1:B:341:THR:HG22 | 1.70 | 0.56 |
| 1:A:400:ASN:OD1 | 1:A:401:LEU:N | 2.38 | 0.56 |
| 1:A:555:ILE:O | 1:A:589:TYR:HD1 | 1.87 | 0.56 |
| 1:A:60:LEU:HD22 | 2:C:671:TYR:CD1 | 2.41 | 0.56 |
| 5:AC:214:SER:OG | 5:AC:222:LEU:O | 2.22 | 0.56 |
| 5:AE:262:GLN:HA | 5:AE:381:ILE:O | 2.06 | 0.56 |
| 1:B:400:ASN:OD1 | 1:B:401:LEU:N | 2.39 | 0.56 |
| 8:BC:10:PHE:C | 8:BC:12:SER:H | 2.08 | 0.56 |
| 9:BD:98:VAL:HB | 9:BD:103:THR:HB | 1.86 | 0.56 |
| 1:BI:189:ASP:HA | 11:DI:121:TYR:HE2 | 1.71 | 0.56 |
| 1:BI:76:TYR:HB3 | 1:BI:82:THR:HG21 | 1.87 | 0.56 |
| 2:BJ:111:GLN:NE2 | 1:EB:646:LEU:O | 2.37 | 0.56 |
| 2:BJ:296:THR:OG1 | 2:BJ:298:ALA:O | 2.23 | 0.56 |
| 2:BJ:800:ARG:HB3 | 2:BJ:809:TRP:CZ3 | 2.40 | 0.56 |
| 2:C:161:SER:O | 2:C:164:SER:N | 2.39 | 0.56 |
| 2:C:10:SER:HB3 | 2:C:26:ASP:HB2 | 1.88 | 0.56 |
| 2:C:420:THR:O | 2:C:424:ARG:NE | 2.38 | 0.56 |
| 2:C:708:ILE:HG13 | 2:C:727:PHE:CD2 | 2.41 | 0.56 |
| 2:C:712:ASN:HD21 | 2:C:720:ARG:HG3 | 1.70 | 0.56 |
| 2:C:741:GLU:OE2 | 2:C:745:LYS:NZ | 2.38 | 0.56 |
| 2:C:808:GLN:NE2 | 2:C:839:ILE:HG13 | 2.21 | 0.56 |
| 3:CA:130:VAL:HG12 | 3:CA:191:LEU:HD12 | 1.86 | 0.56 |
| 4:CD:141:SER:HB3 | 4:CD:164:ILE:HD11 | 1.87 | 0.56 |
| 4:CC:275:ALA:O | 4:CD:282:GLN:NE2 | 2.39 | 0.56 |
| 5:CG:129:ARG:HG3 | 5:CG:130:PHE:H | 1.70 | 0.56 |
| 5:CG:419:ASP:HB3 | 5:CG:436:VAL:HB | 1.86 | 0.56 |
| 5:CH:261:ARG:O | 5:CH:383:ILE:N | 2.37 | 0.56 |
| 3:D:117:ALA:H | 3:D:120:ASN:HB3 | 1.70 | 0.56 |
| 7:DB:439:ILE:HG23 | 7:DD:515:TRP:CH2 | 2.40 | 0.56 |
| 7:DB:440:GLN:OE1 | 7:DB:511:GLU:HG3 | 2.04 | 0.56 |
| 7:DD:49:ASP:HA | 7:DD:57:ILE:O | 2.05 | 0.56 |
| 9:DG:100:ASP:OD1 | 9:DG:101:ASP:N | 2.34 | 0.56 |
| 11:DI:186:ARG:CG | 11:DI:187:ILE:N | 2.68 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:BG:19:ASN:OD1 | 12:DJ:228:LEU:HA | 2.06 | 0.56 |
| 3:E:90:ILE:HG23 | 3:E:210:VAL:HG21 | 1.87 | 0.56 |
| 1:EB:184:PRO:HB2 | 1:EB:186:ILE:HD11 | 1.86 | 0.56 |
| 1:EB:460:ALA:HA | 1:EB:631:VAL:HG12 | 1.87 | 0.56 |
| 4:EH:67:TYR:HD1 | 4:EH:84:ARG:HB3 | 1.70 | 0.56 |
| 5:EI:501:LEU:HD13 | 5:EI:512:PRO:HG2 | 1.88 | 0.56 |
| 5:EJ:313:PHE:CD2 | 5:EJ:320:LEU:HD21 | 2.41 | 0.56 |
| 5:FA:217:GLU:HB2 | 5:FA:222:LEU:HB2 | 1.88 | 0.56 |
| 5:FA:261:ARG:O | 5:FA:383:ILE:N | 2.38 | 0.56 |
| 5:FA:262:GLN:HA | 5:FA:381:ILE:O | 2.05 | 0.56 |
| 6:FB:13:ARG:NH1 | 6:FD:17:PHE:O | 2.31 | 0.56 |
| 7:FF:12:GLU:HG3 | 7:FF:15:TYR:H | 1.71 | 0.56 |
| 12:DJ:126:TYR:HA | 12:GC:230:TYR:CD2 | 2.41 | 0.56 |
| 3:GG:130:VAL:HG12 | 3:GG:191:LEU:HD12 | 1.87 | 0.56 |
| 3:GH:97:ASP:O | 3:GH:103:PRO:HB3 | 2.05 | 0.56 |
| 4:GI:53:GLY:HA3 | 4:GJ:7:LYS:HE2 | 1.88 | 0.56 |
| 5:HB:501:LEU:HD13 | 5:HB:512:PRO:HG2 | 1.88 | 0.56 |
| 5:HB:30:PHE:HE1 | 5:HD:30:PHE:CE1 | 2.23 | 0.56 |
| 5:HD:320:LEU:HD23 | 5:HD:358:VAL:HG23 | 1.87 | 0.56 |
| 7:HI:40:SER:O | 7:HJ:24:ASN:ND2 | 2.37 | 0.56 |
| 5:I:60:LEU:HG | 5:I:79:ILE:HG22 | 1.87 | 0.56 |
| 9:IC:53:PHE:HA | 9:IC:84:TYR:HE2 | 1.70 | 0.56 |
| 5:J:136:VAL:O | 5:J:143:TRP:HA | 2.05 | 0.56 |
| 5:J:313:PHE:CD2 | 5:J:320:LEU:HD21 | 2.41 | 0.56 |
| 5:K:137:TYR:HA | 5:K:143:TRP:CD1 | 2.41 | 0.56 |
| 5:K:237:ASN:OD1 | 5:K:238:ILE:N | 2.38 | 0.56 |
| 7:O:438:GLN:HB2 | 7:Q:516:ASN:OD1 | 2.05 | 0.56 |
| 7:Q:192:GLN:O | 7:Q:208:TYR:HA | 2.05 | 0.56 |
| 7:P:295:ILE:HG13 | 7:Q:301:ARG:HB3 | 1.88 | 0.56 |
| 1:X:246:ASN:ND2 | 1:X:255:ASN:OD1 | 2.39 | 0.56 |
| 1:X:558:PHE:O | 1:X:586:ARG:HB2 | 2.04 | 0.56 |
| 13:YA:265[D]:VAL:HG22 | 13:YA:300[D]:LEU:HD23 | 1.88 | 0.56 |
| 13:YA:527[B]:THR:O | 13:YB:519[B]:THR:HA | 2.06 | 0.56 |
| 13:YA:522[A]:VAL:HA | 13:YB:514[A]:VAL:O | 2.05 | 0.56 |
| 13:YA:522[B]:VAL:HA | 13:YB:514[B]:VAL:O | 2.05 | 0.56 |
| 13:YC:25[D]:GLY:HA3 | 13:YC:73[D]:VAL:HG12 | 1.86 | 0.56 |
| 13:YB:474[C]:ILE:HG12 | 13:YC:466[C]:ASN:HB2 | 1.86 | 0.56 |
| 13:YC:89[F]:LYS:O | 13:YC:91[F]:LYS:HG3 | 2.05 | 0.56 |
| 13:YA:90[A]:TRP:NE1 | 14:YD:175[A]:GLU:OE1 | 2.34 | 0.56 |
| 14:YD:301[E]:MET:HA | 14:YD:304[E]:TYR:HD2 | 1.71 | 0.56 |
| 14:YD:301[F]:MET:HA | 14:YD:304[F]:TYR:HD2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:98[A]:ASP:OD1 | 14:YD:99[A]:SER:N | 2.38 | 0.56 |
| 14:YE:292[D]:TYR:CD1 | 14:YE:371[D]:LYS:HB3 | 2.41 | 0.56 |
| 14:YE:35[A]:ILE:HD11 | 14:YE:38[A]:LEU:HB2 | 1.88 | 0.56 |
| 14:YF:50[B]:GLY:O | 14:YF:109[B]:LEU:N | 2.38 | 0.56 |
| 2:Z:316:ASP:O | 2:Z:331:THR:N | 2.34 | 0.56 |
| 2:Z:36:VAL:HG23 | 2:Z:59:LEU:HB2 | 1.88 | 0.56 |
| 2:Z:420:THR:O | 2:Z:424:ARG:NE | 2.38 | 0.56 |
| 1:A:484:MET:HE1 | 1:A:501:TYR:HB3 | 1.87 | 0.56 |
| 1:A:619:GLN:N | 1:A:619:GLN:OE1 | 2.36 | 0.56 |
| 5:AC:423:THR:O | 7:FG:495:GLN:NE2 | 2.27 | 0.56 |
| 5:AC:594:THR:OG1 | 5:AD:517:GLY:N | 2.38 | 0.56 |
| 5:AD:312:ARG:O | 5:AD:382:ASN:N | 2.30 | 0.56 |
| 5:AD:361:ASP:HB3 | 5:AD:362:GLU:OE1 | 2.06 | 0.56 |
| 5:AC:36:GLU:HG3 | 5:AD:43:PRO:HG2 | 1.88 | 0.56 |
| 5:AE:137:TYR:HA | 5:AE:143:TRP:CD1 | 2.41 | 0.56 |
| 5:AE:339:GLU:HB3 | 6:AF:172:SER:O | 2.05 | 0.56 |
| 6:AF:192:THR:HB | 6:AF:219:ALA:HB3 | 1.87 | 0.56 |
| 7:AI:336:GLU:O | 7:AI:340:THR:N | 2.36 | 0.56 |
| 1:B:90:VAL:HG13 | 1:B:100:PRO:HG3 | 1.87 | 0.56 |
| 8:BB:10:PHE:C | 8:BB:12:SER:H | 2.08 | 0.56 |
| 9:BD:53:PHE:HA | 9:BD:84:TYR:HE2 | 1.70 | 0.56 |
| 12:BG:111:ILE:O | 12:BG:115:ASN:N | 2.28 | 0.56 |
| 1:BI:386:THR:O | 1:BI:389:ARG:N | 2.39 | 0.56 |
| 2:BJ:319:TYR:HD1 | 2:BJ:328:TYR:HB2 | 1.71 | 0.56 |
| 2:C:296:THR:OG1 | 2:C:298:ALA:O | 2.23 | 0.56 |
| 2:C:376:PHE:HB3 | 2:C:405:VAL:HA | 1.86 | 0.56 |
| 2:C:793:CYS:HB3 | 2:C:813:ILE:HG12 | 1.87 | 0.56 |
| 5:CF:501:LEU:HD13 | 5:CF:512:PRO:HG2 | 1.88 | 0.56 |
| 5:CG:193:VAL:HG13 | 5:CG:199:GLU:HB3 | 1.86 | 0.56 |
| 5:CG:313:PHE:CD2 | 5:CG:320:LEU:HD21 | 2.41 | 0.56 |
| 5:CG:322:GLY:N | 5:CG:358:VAL:O | 2.39 | 0.56 |
| 7:DC:310:ASN:OD1 | 7:DC:311:GLY:N | 2.39 | 0.56 |
| 8:DE:55:ASN:HB3 | 8:IA:99:ILE:HD11 | 1.86 | 0.56 |
| 3:E:97:ASP:O | 3:E:103:PRO:HB3 | 2.05 | 0.56 |
| 1:EA:209:TRP:HD1 | 1:EA:225:TYR:HE1 | 1.51 | 0.56 |
| 1:EA:400:ASN:OD1 | 1:EA:401:LEU:N | 2.38 | 0.56 |
| 1:EB:196:GLN:HG3 | 1:EB:273:ILE:HD12 | 1.88 | 0.56 |
| 1:EB:544:ASP:CB | 1:EB:576:ASP:HB2 | 2.36 | 0.56 |
| 3:EE:219:ASP:OD1 | 3:EE:221:THR:N | 2.32 | 0.56 |
| 4:EF:202:LEU:HB3 | 4:EF:278:VAL:HG22 | 1.86 | 0.56 |
| 5:EI:293:PHE:HD1 | 5:EI:298:LEU:HD11 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:36:GLU:HG3 | 5:EJ:43:PRO:HG2 | 1.87 | 0.56 |
| 5:FA:299:ILE:O | 5:FA:301:GLY:N | 2.38 | 0.56 |
| 6:FB:10:VAL:HA | 6:FC:13:ARG:HD2 | 1.88 | 0.56 |
| 6:FC:107:VAL:O | 6:FC:114:VAL:N | 2.38 | 0.56 |
| 6:FB:15:ALA:HB2 | 6:FD:52:ILE:HD11 | 1.88 | 0.56 |
| 7:FE:406:GLY:O | 7:FE:410:THR:HG23 | 2.06 | 0.56 |
| 7:FG:406:GLY:O | 7:FG:410:THR:HG23 | 2.05 | 0.56 |
| 10:GA:39:PRO:HG3 | 10:GA:42:ARG:HH21 | 1.70 | 0.56 |
| 1:GE:184:PRO:HB2 | 1:GE:186:ILE:HD11 | 1.86 | 0.56 |
| 1:GE:582:ASN:HD21 | 1:GE:586:ARG:NH2 | 1.98 | 0.56 |
| 2:GF:19:ASN:OD1 | 2:GF:20:GLN:HG3 | 2.05 | 0.56 |
| 2:GF:10:SER:HB3 | 2:GF:26:ASP:HB2 | 1.88 | 0.56 |
| 2:GF:816:LEU:H | 3:GH:201:ASN:ND2 | 2.04 | 0.56 |
| 4:HA:202:LEU:HA | 4:HA:278:VAL:HA | 1.87 | 0.56 |
| 5:HC:193:VAL:HG13 | 5:HC:199:GLU:HB3 | 1.86 | 0.56 |
| 5:HC:206:PHE:HZ | 5:HC:221:GLU:HG2 | 1.70 | 0.56 |
| 5:HC:361:ASP:HB3 | 5:HC:362:GLU:OE1 | 2.05 | 0.56 |
| 5:HC:290:SER:HA | 5:HC:371:PHE:HB3 | 1.88 | 0.56 |
| 7:HI:99:ARG:HD3 | 7:HI:111:ASN:ND2 | 2.20 | 0.56 |
| 10:ID:237:THR:HA | 10:ID:287:VAL:HG23 | 1.87 | 0.56 |
| 11:IE:131:TYR:O | 11:IE:148:GLY:N | 2.25 | 0.56 |
| 12:IF:218:MET:SD | 12:IF:243:PHE:CD2 | 2.99 | 0.56 |
| 5:I:594:THR:OG1 | 5:J:517:GLY:N | 2.38 | 0.56 |
| 5:K:299:ILE:O | 5:K:301:GLY:N | 2.38 | 0.56 |
| 5:K:415:ASP:HB2 | 5:K:440:GLN:HE22 | 1.71 | 0.56 |
| 5:K:562:SER:C | 5:K:564:PRO:HD3 | 2.26 | 0.56 |
| 7:Q:233:GLN:HE21 | 7:Q:237:ASN:ND2 | 2.04 | 0.56 |
| 8:S:14:ASP:OD2 | 8:S:17:ARG:NH2 | 2.33 | 0.56 |
| 12:W:222:SER:O | 12:W:242:THR:N | 2.39 | 0.56 |
| 13:YA:87[F]:LEU:HD21 | 13:YA:95[F]:ILE:HG23 | 1.86 | 0.56 |
| 13:YA:89[B]:LYS:O | 13:YA:91[B]:LYS:HG3 | 2.06 | 0.56 |
| 13:YB:88[D]:ASP:N | 13:YB:88[D]:ASP:OD1 | 2.38 | 0.56 |
| 14:YD:301[C]:MET:HA | 14:YD:304[C]:TYR:HD2 | 1.71 | 0.56 |
| 14:YD:292[B]:TYR:CD1 | 14:YD:371[B]:LYS:HB3 | 2.41 | 0.56 |
| 14:YD:50[B]:GLY:O | 14:YD:109[B]:LEU:N | 2.38 | 0.56 |
| 14:YE:301[D]:MET:HA | 14:YE:304[D]:TYR:HD2 | 1.71 | 0.56 |
| 14:YE:50[F]:GLY:O | 14:YE:109[F]:LEU:N | 2.38 | 0.56 |
| 14:YE:98[D]:ASP:OD1 | 14:YE:99[D]:SER:N | 2.39 | 0.56 |
| 13:YC:90[F]:TRP:NE1 | 14:YF:175[F]:GLU:OE1 | 2.34 | 0.56 |
| 14:YF:156[E]:TYR:O | 14:YF:177[E]:ALA:HA | 2.06 | 0.56 |
| 14:YF:245[F]:ARG:HD3 | 14:YF:305[F]:ASP:OD2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:292[C]:TYR:CD1 | 14:YF:371[C]:LYS:HB3 | 2.41 | 0.56 |
| 14:YF:301[A]:MET:HA | 14:YF:304[A]:TYR:HD2 | 1.71 | 0.56 |
| 14:YD:101[C]:GLY:HA2 | 14:YF:332[C]:GLN:OE1 | 2.06 | 0.56 |
| 14:YF:50[D]:GLY:O | 14:YF:109[D]:LEU:N | 2.38 | 0.56 |
| 14:YF:98[B]:ASP:OD1 | 14:YF:99[B]:SER:N | 2.39 | 0.56 |
| 2:Z:10:SER:HB3 | 2:Z:26:ASP:HB2 | 1.88 | 0.56 |
| 2:Z:296:THR:OG1 | 2:Z:298:ALA:O | 2.23 | 0.56 |
| 2:Z:458:ASP:OD1 | 2:Z:472:LYS:HB2 | 2.06 | 0.56 |
| 2:Z:982:LEU:O | 2:Z:985:GLU:HB2 | 2.05 | 0.56 |
| 1:A:147:SER:HA | 1:A:167:LEU:HD23 | 1.87 | 0.56 |
| 5:AD:206:PHE:HZ | 5:AD:221:GLU:HG2 | 1.70 | 0.56 |
| 5:AE:261:ARG:O | 5:AE:383:ILE:N | 2.37 | 0.56 |
| 6:AF:73:ASN:HA | 6:AH:70:ILE:HG12 | 1.88 | 0.56 |
| 7:AI:438:GLN:HB2 | 7:BA:516:ASN:OD1 | 2.06 | 0.56 |
| 7:AI:399:PHE:HZ | 7:AI:516:ASN:HD22 | 1.53 | 0.56 |
| 7:AJ:12:GLU:HG3 | 7:AJ:15:TYR:H | 1.71 | 0.56 |
| 7:BA:233:GLN:HE21 | 7:BA:237:ASN:ND2 | 2.04 | 0.56 |
| 11:BF:186:ARG:CG | 11:BF:187:ILE:HG12 | 2.35 | 0.56 |
| 12:BG:222:SER:O | 12:BG:242:THR:N | 2.39 | 0.56 |
| 1:BH:212:LYS:HA | 1:BH:399:TYR:OH | 2.06 | 0.56 |
| 2:BJ:376:PHE:CB | 2:BJ:405:VAL:HA | 2.35 | 0.56 |
| 2:C:1012:LEU:HD13 | 2:C:1027:GLN:OE1 | 2.05 | 0.56 |
| 2:C:146:LEU:HD13 | 2:C:582:ALA:HB1 | 1.87 | 0.56 |
| 3:CB:46:PRO:HA | 3:CB:270:ARG:NH2 | 2.21 | 0.56 |
| 4:CC:39:TYR:CD1 | 4:CD:7:LYS:HB2 | 2.41 | 0.56 |
| 6:CI:73:ASN:HA | 6:DA:70:ILE:HG12 | 1.87 | 0.56 |
| 7:DD:233:GLN:HE21 | 7:DD:237:ASN:ND2 | 2.04 | 0.56 |
| 8:DE:115:GLN:HG2 | 8:FH:79:HIS:HE2 | 1.71 | 0.56 |
| 1:BI:52:ARG:HE | 9:DG:13:PRO:HB3 | 1.70 | 0.56 |
| 12:DJ:218:MET:SD | 12:DJ:243:PHE:CD2 | 2.99 | 0.56 |
| 1:EA:88:SER:O | 1:EA:91:GLN:N | 2.39 | 0.56 |
| 1:EA:400:ASN:H | 1:EB:341:THR:HG22 | 1.70 | 0.56 |
| 2:EC:36:VAL:HG23 | 2:EC:59:LEU:HB2 | 1.88 | 0.56 |
| 2:EC:458:ASP:OD1 | 2:EC:472:LYS:HB2 | 2.06 | 0.56 |
| 5:EJ:73:SER:HB3 | 5:EJ:101:THR:HG21 | 1.87 | 0.56 |
| 5:FA:137:TYR:HA | 5:FA:143:TRP:CD1 | 2.41 | 0.56 |
| 5:FA:196:ARG:NE | 7:FF:5:THR:HG23 | 2.20 | 0.56 |
| 7:FG:386:ASN:OD1 | 7:FG:389:ASN:N | 2.24 | 0.56 |
| 4:G:131:LYS:N | 4:G:160:TRP:O | 2.29 | 0.56 |
| 2:GF:251:ASP:O | 2:GF:301:PRO:HG2 | 2.06 | 0.56 |
| 2:GF:420:THR:O | 2:GF:424:ARG:NE | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:56:PHE:H | 2:GF:467:LEU:HD11 | 1.70 | 0.56 |
| 3:GH:96:GLY:HA2 | 3:GH:104:TYR:CE1 | 2.41 | 0.56 |
| 4:GI:275:ALA:O | 4:GJ:282:GLN:NE2 | 2.39 | 0.56 |
| 5:HB:484:GLY:N | 5:HC:489:GLY:O | 2.28 | 0.56 |
| 5:HD:137:TYR:HA | 5:HD:143:TRP:CD1 | 2.41 | 0.56 |
| 5:HD:168:LEU:HA | 5:HD:241:THR:HG22 | 1.87 | 0.56 |
| 5:HD:36:GLU:HA | 5:HD:50:LYS:HZ1 | 1.71 | 0.56 |
| 5:I:118:LYS:NZ | 5:I:145:TYR:O | 2.37 | 0.56 |
| 5:I:391:GLY:O | 5:I:392:THR:OG1 | 2.23 | 0.56 |
| 8:IA:10:PHE:C | 8:IA:12:SER:H | 2.08 | 0.56 |
| 11:IE:186:ARG:CG | 11:IE:187:ILE:HG12 | 2.35 | 0.56 |
| 5:J:361:ASP:HB3 | 5:J:362:GLU:OE1 | 2.06 | 0.56 |
| 5:J:503:ASN:OD1 | 5:J:504:ASN:ND2 | 2.38 | 0.56 |
| 5:J:9:ASN:OD1 | 5:J:10:VAL:N | 2.39 | 0.56 |
| 5:K:217:GLU:HB2 | 5:K:222:LEU:HB2 | 1.88 | 0.56 |
| 7:P:99:ARG:HD3 | 7:P:111:ASN:ND2 | 2.20 | 0.56 |
| 7:Q:89:ASN:OD1 | 7:Q:90:ALA:N | 2.39 | 0.56 |
| 10:U:237:THR:HA | 10:U:287:VAL:HG23 | 1.87 | 0.56 |
| 1:Y:647:ARG:HD3 | 1:Y:650:TYR:HE2 | 1.71 | 0.56 |
| 13:YA:214[D]:MET:HG2 | 13:YA:232[D]:ASN:O | 2.06 | 0.56 |
| 13:YA:527[F]:THR:O | 13:YB:519[F]:THR:HA | 2.05 | 0.56 |
| 13:YB:321[D]:LYS:HG2 | 13:YC:453[D]:ASP:OD1 | 2.05 | 0.56 |
| 13:YB:89[D]:LYS:O | 13:YB:91[D]:LYS:HG3 | 2.06 | 0.56 |
| 13:YC:265[F]:VAL:HG22 | 13:YC:300[F]:LEU:HD23 | 1.88 | 0.56 |
| 13:YB:572[F]:ILE:HA | 13:YC:565[F]:TYR:O | 2.06 | 0.56 |
| 14:YD:50[E]:GLY:O | 14:YD:109[E]:LEU:N | 2.38 | 0.56 |
| 14:YD:98[C]:ASP:OD1 | 14:YD:99[C]:SER:N | 2.39 | 0.56 |
| 14:YD:92[B]:HIS:NE2 | 14:YF:238[B]:THR:OG1 | 2.39 | 0.56 |
| 14:YF:292[B]:TYR:CD1 | 14:YF:371[B]:LYS:HB3 | 2.41 | 0.56 |
| 14:YE:238[F]:THR:OG1 | 14:YF:92[F]:HIS:NE2 | 2.39 | 0.56 |
| 2:Z:143:MET:HG2 | 2:Z:544:VAL:HG22 | 1.88 | 0.56 |
| 2:Z:351:GLU:CB | 2:Z:353:ASP:HB2 | 2.31 | 0.56 |
| 1:A:423:THR:O | 1:A:476:ILE:N | 2.35 | 0.56 |
| 7:AJ:236:VAL:HG21 | 7:AJ:249:THR:HB | 1.88 | 0.56 |
| 7:AJ:310:ASN:OD1 | 7:AJ:311:GLY:N | 2.39 | 0.56 |
| 10:BE:285:LEU:HA | 14:YF:215[E]:GLU:CG | 2.36 | 0.56 |
| 2:BJ:10:SER:HB3 | 2:BJ:26:ASP:HB2 | 1.88 | 0.56 |
| 2:BJ:376:PHE:HB3 | 2:BJ:405:VAL:HA | 1.86 | 0.56 |
| 2:C:36:VAL:HG23 | 2:C:59:LEU:HB2 | 1.88 | 0.56 |
| 3:CB:90:ILE:HG23 | 3:CB:210:VAL:HG21 | 1.87 | 0.56 |
| 4:CC:202:LEU:HA | 4:CC:278:VAL:HA | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CC:67:TYR:HD1 | 4:CC:84:ARG:HB3 | 1.70 | 0.56 |
| 4:CD:1:MET:HG2 | 4:CD:70:HIS:CE1 | 2.41 | 0.56 |
| 5:CF:293:PHE:HD1 | 5:CF:298:LEU:HD11 | 1.71 | 0.56 |
| 5:CF:326:MET:HE3 | 5:CG:279:SER:HB2 | 1.87 | 0.56 |
| 5:CH:137:TYR:HA | 5:CH:143:TRP:CD1 | 2.41 | 0.56 |
| 5:CH:212:PHE:CZ | 5:CH:230:ILE:HB | 2.41 | 0.56 |
| 10:DH:39:PRO:HG3 | 10:DH:42:ARG:HH21 | 1.70 | 0.56 |
| 2:EC:422:GLU:HB3 | 2:EC:423:GLU:OE1 | 2.06 | 0.56 |
| 3:ED:204:THR:HG21 | 3:ED:248:ARG:HH22 | 1.69 | 0.56 |
| 4:EG:154:ASP:HB2 | 4:EG:157:THR:HB | 1.88 | 0.56 |
| 4:EG:202:LEU:HA | 4:EG:278:VAL:HA | 1.87 | 0.56 |
| 5:EI:326:MET:CE | 5:EJ:264:ARG:HB3 | 2.36 | 0.56 |
| 5:EJ:9:ASN:OD1 | 5:EJ:10:VAL:N | 2.39 | 0.56 |
| 5:FA:398:GLU:OE1 | 5:FA:398:GLU:N | 2.37 | 0.56 |
| 7:FF:394:ASP:OD2 | 7:FG:407:SER:N | 2.29 | 0.56 |
| 7:FG:192:GLN:O | 7:FG:208:TYR:HA | 2.05 | 0.56 |
| 7:FG:233:GLN:HE21 | 7:FG:237:ASN:ND2 | 2.04 | 0.56 |
| 10:GA:129:LEU:HD13 | 10:GA:209:TRP:HZ3 | 1.70 | 0.56 |
| 12:GC:217:THR:O | 12:GC:246:ARG:N | 2.32 | 0.56 |
| 2:GF:125:GLU:HG2 | 2:GF:134:TYR:CG | 2.41 | 0.56 |
| 1:GE:52:ARG:HD3 | 2:GF:657:TYR:HD1 | 1.69 | 0.56 |
| 2:GF:793:CYS:HB3 | 2:GF:813:ILE:HG12 | 1.87 | 0.56 |
| 5:HB:293:PHE:HD1 | 5:HB:298:LEU:HD11 | 1.71 | 0.56 |
| 5:HB:330:HIS:ND1 | 5:HB:355:ASP:HB2 | 2.21 | 0.56 |
| 5:HD:507:ASP:OD1 | 5:HD:511:ASN:N | 2.25 | 0.56 |
| 7:HH:406:GLY:O | 7:HH:410:THR:HG23 | 2.05 | 0.56 |
| 7:HI:214:THR:HA | 7:HI:217:ASN:HD21 | 1.70 | 0.56 |
| 7:HI:476:ASP:CG | 7:HI:479:ASN:HD21 | 2.09 | 0.56 |
| 5:I:252:SER:OG | 5:I:393:LEU:HB3 | 2.05 | 0.56 |
| 6:L:192:THR:HB | 6:L:219:ALA:HB3 | 1.87 | 0.56 |
| 7:P:466:SER:HB3 | 7:P:468:PHE:HE2 | 1.71 | 0.56 |
| 13:YA:57[E]:VAL:HG11 | 13:YA:75[E]:GLY:HA3 | 1.88 | 0.56 |
| 13:YA:82[E]:VAL:HG22 | 13:YA:98[E]:GLY:O | 2.05 | 0.56 |
| 13:YB:416[B]:HIS:HD2 | 13:YB:418[B]:THR:H | 1.52 | 0.56 |
| 13:YB:82[B]:VAL:HG22 | 13:YB:98[B]:GLY:O | 2.05 | 0.56 |
| 13:YB:89[F]:LYS:O | 13:YB:91[F]:LYS:HG3 | 2.05 | 0.56 |
| 13:YB:89[B]:LYS:O | 13:YB:91[B]:LYS:HG3 | 2.06 | 0.56 |
| 13:YC:293[F]:ASN:O | 13:YC:297[F]:THR:N | 2.39 | 0.56 |
| 14:YD:292[A]:TYR:CD1 | 14:YD:371[A]:LYS:HB3 | 2.41 | 0.56 |
| 14:YD:189[E]:TRP:NE1 | 14:YD:320[E]:PRO:HG2 | 2.21 | 0.56 |
| 14:YD:332[C]:GLN:OE1 | 14:YE:101[C]:GLY:HA2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:245[E]:ARG:HD3 | 14:YE:305[E]:ASP:OD2 | 2.06 | 0.56 |
| 14:YE:292[E]:TYR:CD1 | 14:YE:371[E]:LYS:HB3 | 2.41 | 0.56 |
| 14:YE:50[C]:GLY:O | 14:YE:109[C]:LEU:N | 2.38 | 0.56 |
| 14:YE:50[E]:GLY:O | 14:YE:109[E]:LEU:N | 2.38 | 0.56 |
| 14:YF:189[A]:TRP:NE1 | 14:YF:320[A]:PRO:HG2 | 2.21 | 0.56 |
| 14:YF:301[E]:MET:HA | 14:YF:304[E]:TYR:HD2 | 1.71 | 0.56 |
| 2:Z:738:LYS:HD2 | 2:Z:882:PHE:O | 2.06 | 0.56 |
| 1:A:212:LYS:HA | 1:A:399:TYR:OH | 2.05 | 0.56 |
| 1:A:246:ASN:ND2 | 1:A:255:ASN:OD1 | 2.39 | 0.56 |
| 4:AB:131:LYS:N | 4:AB:160:TRP:O | 2.29 | 0.56 |
| 5:AC:371:PHE:CZ | 5:AC:373:SER:HB3 | 2.41 | 0.56 |
| 5:AD:326:MET:HE1 | 5:AE:264:ARG:H | 1.69 | 0.56 |
| 5:AD:503:ASN:OD1 | 5:AD:504:ASN:ND2 | 2.38 | 0.56 |
| 1:B:213:SER:OG | 1:B:337:GLN:OE1 | 2.23 | 0.56 |
| 1:B:386:THR:O | 1:B:389:ARG:N | 2.39 | 0.56 |
| 7:BA:383:TYR:CD1 | 7:BA:393:PRO:HG3 | 2.41 | 0.56 |
| 7:BA:453:GLU:OE2 | 7:BA:471:THR:N | 2.29 | 0.56 |
| 12:BG:149:ARG:HB2 | 10:DH:341:THR:HG21 | 1.87 | 0.56 |
| 1:BH:448:TYR:CZ | 1:BH:642:PHE:HB2 | 2.41 | 0.56 |
| 1:BH:619:GLN:OE1 | 1:BH:619:GLN:N | 2.36 | 0.56 |
| 1:BH:9:GLN:OE1 | 1:BH:9:GLN:N | 2.39 | 0.56 |
| 1:BI:196:GLN:HG3 | 1:BI:273:ILE:HD12 | 1.88 | 0.56 |
| 2:C:20:GLN:HA | 2:C:70:ASP:HA | 1.87 | 0.56 |
| 3:CA:204:THR:HG21 | 3:CA:248:ARG:HH22 | 1.69 | 0.56 |
| 4:CE:1:MET:HG2 | 4:CE:70:HIS:CE1 | 2.41 | 0.56 |
| 5:CG:290:SER:CB | 5:CG:370:HIS:HA | 2.35 | 0.56 |
| 5:CG:9:ASN:OD1 | 5:CG:10:VAL:N | 2.39 | 0.56 |
| 5:CH:262:GLN:HA | 5:CH:381:ILE:O | 2.05 | 0.56 |
| 7:DD:89:ASN:OD1 | 7:DD:90:ALA:N | 2.39 | 0.56 |
| 2:C:768:TYR:CG | 3:E:197:ASP:HB3 | 2.41 | 0.56 |
| 1:EA:145:PHE:CZ | 1:EA:286:PHE:HE1 | 2.24 | 0.56 |
| 1:EB:582:ASN:HD21 | 1:EB:586:ARG:NH2 | 1.98 | 0.56 |
| 2:EC:125:GLU:HG2 | 2:EC:134:TYR:CG | 2.41 | 0.56 |
| 2:EC:433:ASN:O | 2:EC:443:LEU:HA | 2.06 | 0.56 |
| 2:EC:146:LEU:HD13 | 2:EC:582:ALA:HB1 | 1.87 | 0.56 |
| 4:EH:1:MET:HG2 | 4:EH:70:HIS:CE1 | 2.41 | 0.56 |
| 5:EI:330:HIS:ND1 | 5:EI:355:ASP:HB2 | 2.21 | 0.56 |
| 5:EI:569:TYR:CD1 | 5:EJ:544:VAL:HA | 2.41 | 0.56 |
| 5:EJ:322:GLY:N | 5:EJ:358:VAL:O | 2.39 | 0.56 |
| 5:FA:320:LEU:HD23 | 5:FA:358:VAL:HG23 | 1.87 | 0.56 |
| 6:FC:192:THR:HB | 6:FC:219:ALA:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:202:LEU:HA | 4:G:278:VAL:HA | 1.87 | 0.56 |
| 1:GE:213:SER:OG | 1:GE:337:GLN:OE1 | 2.23 | 0.56 |
| 1:GD:400:ASN:H | 1:GE:341:THR:HG22 | 1.71 | 0.56 |
| 2:GF:316:ASP:O | 2:GF:331:THR:N | 2.34 | 0.56 |
| 4:GJ:202:LEU:HA | 4:GJ:278:VAL:HA | 1.87 | 0.56 |
| 5:HC:322:GLY:N | 5:HC:358:VAL:O | 2.39 | 0.56 |
| 5:HD:562:SER:C | 5:HD:564:PRO:HD3 | 2.26 | 0.56 |
| 7:HH:497:ASN:H | 7:HH:500:TYR:HB2 | 1.71 | 0.56 |
| 5:I:501:LEU:HD13 | 5:I:512:PRO:HG2 | 1.88 | 0.56 |
| 8:S:139:GLU:H | 8:IB:43:ALA:HB2 | 1.71 | 0.56 |
| 5:J:312:ARG:O | 5:J:382:ASN:N | 2.30 | 0.56 |
| 5:I:484:GLY:N | 5:J:489:GLY:O | 2.29 | 0.56 |
| 5:I:255:ARG:NE | 5:K:390:LEU:HD12 | 2.20 | 0.56 |
| 7:O:146:SER:O | 7:O:150:ALA:N | 2.38 | 0.56 |
| 8:S:10:PHE:C | 8:S:12:SER:H | 2.08 | 0.56 |
| 12:W:22:PHE:HA | 12:W:203:LEU:HA | 1.86 | 0.56 |
| 1:X:388:GLN:O | 1:X:392:ILE:HG22 | 2.06 | 0.56 |
| 1:X:9:GLN:OE1 | 1:X:9:GLN:N | 2.39 | 0.56 |
| 1:Y:148:ARG:NH2 | 1:Y:196:GLN:HE22 | 2.04 | 0.56 |
| 13:YC:214[F]:MET:HG2 | 13:YC:232[F]:ASN:O | 2.06 | 0.56 |
| 13:YC:26[E]:ARG:HA | 13:YC:55[E]:MET:O | 2.05 | 0.56 |
| 14:YD:301[B]:MET:HA | 14:YD:304[B]:TYR:HD2 | 1.71 | 0.56 |
| 14:YD:245[D]:ARG:HD3 | 14:YD:305[D]:ASP:OD2 | 2.06 | 0.56 |
| 14:YD:292[C]:TYR:CD1 | 14:YD:371[C]:LYS:HB3 | 2.41 | 0.56 |
| 14:YD:292[F]:TYR:CD1 | 14:YD:371[F]:LYS:HB3 | 2.42 | 0.56 |
| 14:YE:156[A]:TYR:O | 14:YE:177[A]:ALA:HA | 2.06 | 0.56 |
| 14:YE:245[F]:ARG:HD3 | 14:YE:305[F]:ASP:OD2 | 2.06 | 0.56 |
| 14:YE:64[D]:MET:HE3 | 14:YE:68[D]:GLU:HG3 | 1.87 | 0.56 |
| 13:YC:90[B]:TRP:NE1 | 14:YF:175[B]:GLU:OE1 | 2.35 | 0.56 |
| 1:A:303:ASN:ND2 | 1:A:310:PHE:CE2 | 2.74 | 0.55 |
| 4:AA:141:SER:HB3 | 4:AA:164:ILE:HD11 | 1.87 | 0.55 |
| 4:AA:67:TYR:HD1 | 4:AA:84:ARG:HB3 | 1.70 | 0.55 |
| 5:AC:103:ASN:OD1 | 5:AC:104:VAL:N | 2.39 | 0.55 |
| 5:AC:252:SER:OG | 5:AC:393:LEU:HB3 | 2.06 | 0.55 |
| 5:AC:326:MET:HE3 | 5:AD:279:SER:HB2 | 1.88 | 0.55 |
| 5:AD:73:SER:HB3 | 5:AD:101:THR:HG21 | 1.87 | 0.55 |
| 5:AE:217:GLU:HB2 | 5:AE:222:LEU:HB2 | 1.88 | 0.55 |
| 5:AE:353:HIS:NE2 | 7:FG:476:ASP:HB2 | 2.20 | 0.55 |
| 5:AE:562:SER:C | 5:AE:564:PRO:HD3 | 2.26 | 0.55 |
| 7:AJ:418:ASP:OD1 | 7:AJ:422:LYS:N | 2.38 | 0.55 |
| 7:AJ:466:SER:HB3 | 7:AJ:468:PHE:HE2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BA:194:ALA:HB2 | 7:BA:208:TYR:HB3 | 1.88 | 0.55 |
| 7:AI:199:VAL:HG12 | 7:BA:212:PRO:HG3 | 1.86 | 0.55 |
| 7:BA:89:ASN:OD1 | 7:BA:90:ALA:N | 2.39 | 0.55 |
| 2:BJ:433:ASN:O | 2:BJ:443:LEU:HA | 2.06 | 0.55 |
| 5:CF:103:ASN:OD1 | 5:CF:104:VAL:N | 2.39 | 0.55 |
| 5:CF:330:HIS:ND1 | 5:CF:355:ASP:HB2 | 2.21 | 0.55 |
| 5:CF:36:GLU:HG3 | 5:CG:43:PRO:HG2 | 1.88 | 0.55 |
| 5:CH:18:TYR:HB2 | 5:CH:21:LYS:H | 1.71 | 0.55 |
| 5:CH:320:LEU:HD23 | 5:CH:358:VAL:HG23 | 1.87 | 0.55 |
| 6:CI:13:ARG:HB2 | 6:DA:10:VAL:HA | 1.87 | 0.55 |
| 7:DC:236:VAL:HG21 | 7:DC:249:THR:HB | 1.88 | 0.55 |
| 5:CH:196:ARG:NE | 7:DC:5:THR:HG23 | 2.21 | 0.55 |
| 7:DD:330:ARG:NH2 | 7:DD:336:GLU:OE2 | 2.39 | 0.55 |
| 7:DD:392:LEU:HD22 | 7:DD:523:ILE:HG21 | 1.89 | 0.55 |
| 1:EA:246:ASN:ND2 | 1:EA:255:ASN:OD1 | 2.39 | 0.55 |
| 2:EC:206:GLN:HG3 | 5:FA:555:CYS:O | 2.07 | 0.55 |
| 2:EC:319:TYR:HD1 | 2:EC:328:TYR:HB2 | 1.71 | 0.55 |
| 2:EC:712:ASN:HD21 | 2:EC:720:ARG:HG3 | 1.70 | 0.55 |
| 3:EE:29:GLY:HA3 | 3:EE:34:LYS:HB2 | 1.88 | 0.55 |
| 3:EE:96:GLY:HA2 | 3:EE:104:TYR:CE1 | 2.41 | 0.55 |
| 3:EE:97:ASP:O | 3:EE:103:PRO:HB3 | 2.05 | 0.55 |
| 4:EF:67:TYR:HD1 | 4:EF:84:ARG:HB3 | 1.70 | 0.55 |
| 4:EG:42:PHE:O | 4:EG:62:HIS:ND1 | 2.27 | 0.55 |
| 5:EI:146:VAL:HG21 | 5:EJ:153:LYS:HD3 | 1.88 | 0.55 |
| 5:EI:371:PHE:CZ | 5:EI:373:SER:HB3 | 2.41 | 0.55 |
| 5:FA:185:SER:HB2 | 5:FA:228:PHE:HE1 | 1.72 | 0.55 |
| 5:EJ:317:LEU:HD13 | 5:FA:312:ARG:NH2 | 2.21 | 0.55 |
| 7:FF:295:ILE:HG13 | 7:FG:301:ARG:HB3 | 1.86 | 0.55 |
| 7:FE:359:TRP:NE1 | 7:FF:340:THR:O | 2.27 | 0.55 |
| 8:FI:14:ASP:OD2 | 8:FI:17:ARG:NH2 | 2.33 | 0.55 |
| 1:GD:303:ASN:ND2 | 1:GD:310:PHE:CE2 | 2.74 | 0.55 |
| 1:GD:88:SER:O | 1:GD:91:GLN:N | 2.39 | 0.55 |
| 1:GE:460:ALA:HA | 1:GE:631:VAL:HG12 | 1.87 | 0.55 |
| 2:GF:143:MET:HG2 | 2:GF:544:VAL:HG22 | 1.87 | 0.55 |
| 2:GF:36:VAL:HG23 | 2:GF:59:LEU:HB2 | 1.88 | 0.55 |
| 2:GF:708:ILE:HG13 | 2:GF:727:PHE:CD2 | 2.41 | 0.55 |
| 4:GI:1:MET:HG2 | 4:GI:70:HIS:CE1 | 2.41 | 0.55 |
| 4:H:202:LEU:HA | 4:H:278:VAL:HA | 1.87 | 0.55 |
| 5:HC:202:TYR:OH | 5:HC:223:VAL:O | 2.19 | 0.55 |
| 5:HB:326:MET:CE | 5:HC:264:ARG:HB3 | 2.35 | 0.55 |
| 5:HC:313:PHE:CD2 | 5:HC:320:LEU:HD21 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:308:SER:HG | 5:HD:258:TYR:HD2 | 1.51 | 0.55 |
| 5:HB:356:TYR:CE1 | 6:HG:4:LEU:HD13 | 2.41 | 0.55 |
| 5:J:322:GLY:N | 5:J:358:VAL:O | 2.39 | 0.55 |
| 7:O:406:GLY:O | 7:O:410:THR:HG23 | 2.06 | 0.55 |
| 1:B:189:ASP:HA | 11:V:121:TYR:HE2 | 1.71 | 0.55 |
| 12:W:111:ILE:O | 12:W:115:ASN:N | 2.28 | 0.55 |
| 13:YA:26[B]:ARG:HA | 13:YA:55[B]:MET:O | 2.06 | 0.55 |
| 13:YA:265[B]:VAL:HG22 | 13:YA:300[B]:LEU:HD23 | 1.88 | 0.55 |
| 13:YA:83[E]:TYR:CZ | 13:YC:95[E]:ILE:HD11 | 2.41 | 0.55 |
| 13:YA:89[D]:LYS:O | 13:YA:91[D]:LYS:HG3 | 2.06 | 0.55 |
| 13:YB:321[C]:LYS:HG2 | 13:YC:453[C]:ASP:OD1 | 2.05 | 0.55 |
| 13:YC:214[A]:MET:HG2 | 13:YC:232[A]:ASN:O | 2.06 | 0.55 |
| 1:A:526:PRO:HB3 | 13:YC:254[E]:ARG:HD3 | 1.87 | 0.55 |
| 13:YB:321[B]:LYS:HG2 | 13:YC:453[B]:ASP:OD1 | 2.05 | 0.55 |
| 13:YC:57[E]:VAL:HG11 | 13:YC:75[E]:GLY:HA3 | 1.88 | 0.55 |
| 13:YC:82[B]:VAL:HG22 | 13:YC:98[B]:GLY:O | 2.05 | 0.55 |
| 14:YD:156[C]:TYR:O | 14:YD:177[C]:ALA:HA | 2.07 | 0.55 |
| 14:YD:156[F]:TYR:O | 14:YD:177[F]:ALA:HA | 2.06 | 0.55 |
| 14:YD:178[D]:LEU:HD11 | 14:YD:183[D]:ASP:HA | 1.88 | 0.55 |
| 14:YD:245[A]:ARG:HD3 | 14:YD:305[A]:ASP:OD2 | 2.06 | 0.55 |
| 14:YD:64[C]:MET:HE3 | 14:YD:68[C]:GLU:HG3 | 1.87 | 0.55 |
| 14:YE:189[D]:TRP:NE1 | 14:YE:320[D]:PRO:HG2 | 2.21 | 0.55 |
| 14:YE:301[A]:MET:HA | 14:YE:304[A]:TYR:HD2 | 1.71 | 0.55 |
| 14:YE:292[F]:TYR:CD1 | 14:YE:371[F]:LYS:HB3 | 2.42 | 0.55 |
| 14:YE:64[B]:MET:HE3 | 14:YE:68[B]:GLU:HG3 | 1.87 | 0.55 |
| 14:YF:50[A]:GLY:O | 14:YF:109[A]:LEU:N | 2.38 | 0.55 |
| 14:YF:245[C]:ARG:HD3 | 14:YF:305[C]:ASP:OD2 | 2.06 | 0.55 |
| 14:YF:50[C]:GLY:O | 14:YF:109[C]:LEU:N | 2.38 | 0.55 |
| 14:YF:64[A]:MET:HE3 | 14:YF:68[A]:GLU:HG3 | 1.87 | 0.55 |
| 14:YF:64[E]:MET:HE3 | 14:YF:68[E]:GLU:HG3 | 1.87 | 0.55 |
| 2:Z:517:SER:O | 2:Z:521:ASN:HA | 2.06 | 0.55 |
| 2:Z:712:ASN:HD21 | 2:Z:720:ARG:HG3 | 1.70 | 0.55 |
| 2:Z:825:GLU:N | 2:Z:837:GLU:OE1 | 2.40 | 0.55 |
| 5:AD:317:LEU:HD13 | 5:AE:312:ARG:NH2 | 2.21 | 0.55 |
| 5:AD:322:GLY:N | 5:AD:358:VAL:O | 2.39 | 0.55 |
| 5:AE:316:ILE:HG21 | 6:AG:7:LYS:HG3 | 1.88 | 0.55 |
| 5:AE:415:ASP:HB2 | 5:AE:440:GLN:HE22 | 1.71 | 0.55 |
| 6:AG:23:LYS:HB3 | 6:AG:26:ASP:HB2 | 1.89 | 0.55 |
| 1:B:455:PHE:HD2 | 1:B:456:ASN:HB2 | 1.71 | 0.55 |
| 1:B:70:PHE:HE2 | 2:C:686:LEU:CB | 2.17 | 0.55 |
| 1:B:76:TYR:HB3 | 1:B:82:THR:HG21 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BA:54:THR:HG22 | 7:BA:55:LYS:O | 2.05 | 0.55 |
| 11:BF:17:ASN:ND2 | 11:BF:19:ASN:O | 2.39 | 0.55 |
| 2:BJ:125:GLU:HG2 | 2:BJ:134:TYR:CG | 2.41 | 0.55 |
| 2:C:251:ASP:O | 2:C:301:PRO:HG2 | 2.06 | 0.55 |
| 2:C:935:LYS:HZ3 | 2:C:936:LEU:HD13 | 1.71 | 0.55 |
| 4:CD:154:ASP:HB2 | 4:CD:157:THR:HB | 1.88 | 0.55 |
| 5:CF:156:SER:HB3 | 5:CG:154:ILE:HG12 | 1.87 | 0.55 |
| 5:CF:358:VAL:HA | 5:CF:371:PHE:HA | 1.86 | 0.55 |
| 6:CJ:107:VAL:O | 6:CJ:114:VAL:N | 2.37 | 0.55 |
| 6:DA:192:THR:HB | 6:DA:219:ALA:HB3 | 1.87 | 0.55 |
| 7:DB:289:GLN:OE1 | 7:DB:294:GLN:NE2 | 2.39 | 0.55 |
| 7:DB:447:HIS:CD2 | 7:DC:447:HIS:CD2 | 2.93 | 0.55 |
| 12:BG:153:ARG:HH12 | 12:DJ:184:PRO:HA | 1.71 | 0.55 |
| 1:EA:147:SER:HA | 1:EA:167:LEU:HD23 | 1.88 | 0.55 |
| 1:EA:341:THR:HG22 | 1:EA:343:THR:H | 1.71 | 0.55 |
| 1:EB:455:PHE:HD2 | 1:EB:456:ASN:HB2 | 1.72 | 0.55 |
| 2:EC:808:GLN:NE2 | 2:EC:839:ILE:HG13 | 2.21 | 0.55 |
| 3:EE:46:PRO:HA | 3:EE:270:ARG:NH2 | 2.21 | 0.55 |
| 4:EG:202:LEU:HB3 | 4:EG:278:VAL:HG22 | 1.86 | 0.55 |
| 5:EI:356:TYR:CE1 | 6:FD:4:LEU:HD13 | 2.41 | 0.55 |
| 5:EI:60:LEU:HG | 5:EI:79:ILE:HG22 | 1.87 | 0.55 |
| 4:F:1:MET:HG2 | 4:F:70:HIS:CE1 | 2.41 | 0.55 |
| 4:G:1:MET:HG2 | 4:G:70:HIS:CE1 | 2.41 | 0.55 |
| 1:GD:339:CYS:HB3 | 1:GD:348:PHE:CE2 | 2.42 | 0.55 |
| 1:GE:148:ARG:NH2 | 1:GE:196:GLN:HE22 | 2.03 | 0.55 |
| 4:GJ:202:LEU:HB3 | 4:GJ:278:VAL:HG22 | 1.86 | 0.55 |
| 4:H:141:SER:HB3 | 4:H:164:ILE:HD11 | 1.87 | 0.55 |
| 5:HB:194:LYS:HE3 | 5:HD:198:ASN:HD22 | 1.69 | 0.55 |
| 5:HB:419:ASP:HB3 | 5:HB:436:VAL:HB | 1.88 | 0.55 |
| 5:HC:129:ARG:HG3 | 5:HC:130:PHE:H | 1.70 | 0.55 |
| 5:HD:31:ASP:O | 5:HD:35:TYR:N | 2.27 | 0.55 |
| 7:HI:236:VAL:HG21 | 7:HI:249:THR:HB | 1.88 | 0.55 |
| 7:HH:301:ARG:HB3 | 7:HJ:295:ILE:HG13 | 1.88 | 0.55 |
| 11:IE:36:PHE:HZ | 11:IE:76:CYS:HG | 1.51 | 0.55 |
| 5:J:285:LEU:HD11 | 5:J:375:PHE:CB | 2.28 | 0.55 |
| 5:K:18:TYR:HB2 | 5:K:21:LYS:H | 1.71 | 0.55 |
| 5:K:312:ARG:O | 5:K:382:ASN:N | 2.25 | 0.55 |
| 7:O:297:TYR:HB2 | 7:Q:291:ARG:HA | 1.88 | 0.55 |
| 7:P:214:THR:HA | 7:P:217:ASN:HD21 | 1.70 | 0.55 |
| 7:P:236:VAL:HG21 | 7:P:249:THR:HB | 1.88 | 0.55 |
| 7:P:192:GLN:NE2 | 7:Q:185:GLU:O | 2.33 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:279:ASP:OD1 | 1:Y:280:ALA:N | 2.39 | 0.55 |
| 13:YA:293[D]:ASN:O | 13:YA:297[D]:THR:N | 2.40 | 0.55 |
| 13:YA:442[C]:THR:HG21 | 13:YB:438[C]:LEU:HD22 | 1.88 | 0.55 |
| 13:YA:9[A]:ASN:HA | 13:YC:7[A]:ASN:ND2 | 2.17 | 0.55 |
| 13:YB:214[C]:MET:HG2 | 13:YB:232[C]:ASN:O | 2.06 | 0.55 |
| 13:YB:214[B]:MET:HG2 | 13:YB:232[B]:ASN:O | 2.06 | 0.55 |
| 13:YB:265[F]:VAL:HG22 | 13:YB:300[F]:LEU:HD23 | 1.88 | 0.55 |
| 13:YA:503[F]:THR:O | 13:YB:495[F]:THR:HA | 2.06 | 0.55 |
| 13:YC:265[D]:VAL:HG22 | 13:YC:300[D]:LEU:HD23 | 1.88 | 0.55 |
| 13:YC:87[E]:LEU:HD21 | 13:YC:95[E]:ILE:HG23 | 1.87 | 0.55 |
| 13:YC:89[D]:LYS:O | 13:YC:91[D]:LYS:HG3 | 2.06 | 0.55 |
| 13:YC:89[E]:LYS:O | 13:YC:91[E]:LYS:HG3 | 2.06 | 0.55 |
| 14:YD:50[A]:GLY:O | 14:YD:109[A]:LEU:N | 2.38 | 0.55 |
| 14:YE:156[D]:TYR:O | 14:YE:177[D]:ALA:HA | 2.07 | 0.55 |
| 14:YE:245[B]:ARG:HD3 | 14:YE:305[B]:ASP:OD2 | 2.06 | 0.55 |
| 11:DI:190:LYS:HE3 | 14:YE:24[C]:SER:O | 2.04 | 0.55 |
| 14:YE:292[A]:TYR:CD1 | 14:YE:371[A]:LYS:HB3 | 2.41 | 0.55 |
| 14:YF:292[E]:TYR:CD1 | 14:YF:371[E]:LYS:HB3 | 2.41 | 0.55 |
| 14:YF:301[D]:MET:HA | 14:YF:304[D]:TYR:HD2 | 1.71 | 0.55 |
| 14:YF:245[D]:ARG:HD3 | 14:YF:305[D]:ASP:OD2 | 2.06 | 0.55 |
| 2:Z:251:ASP:O | 2:Z:301:PRO:HG2 | 2.06 | 0.55 |
| 4:AA:154:ASP:HB2 | 4:AA:157:THR:HB | 1.88 | 0.55 |
| 4:AB:1:MET:HG2 | 4:AB:70:HIS:CE1 | 2.41 | 0.55 |
| 5:AC:63:GLU:HB2 | 5:AC:68:TYR:OH | 2.07 | 0.55 |
| 5:AD:313:PHE:CD2 | 5:AD:320:LEU:HD21 | 2.41 | 0.55 |
| 5:AE:60:LEU:HG | 5:AE:79:ILE:HG22 | 1.88 | 0.55 |
| 7:AI:439:ILE:HG23 | 7:BA:515:TRP:CH2 | 2.42 | 0.55 |
| 5:AC:196:ARG:HH11 | 7:AI:5:THR:HG23 | 1.70 | 0.55 |
| 7:AJ:211:SER:N | 7:AJ:214:THR:OG1 | 2.28 | 0.55 |
| 1:B:148:ARG:NH2 | 1:B:196:GLN:HE22 | 2.04 | 0.55 |
| 1:B:279:ASP:OD1 | 1:B:280:ALA:N | 2.39 | 0.55 |
| 1:B:544:ASP:CB | 1:B:576:ASP:HB2 | 2.36 | 0.55 |
| 1:B:647:ARG:HD3 | 1:B:650:TYR:HE2 | 1.71 | 0.55 |
| 7:BA:49:ASP:HA | 7:BA:57:ILE:O | 2.05 | 0.55 |
| 12:BG:218:MET:SD | 12:BG:243:PHE:CD2 | 2.99 | 0.55 |
| 1:BH:246:ASN:ND2 | 1:BH:255:ASN:OD1 | 2.39 | 0.55 |
| 1:BH:303:ASN:ND2 | 1:BH:310:PHE:CE2 | 2.74 | 0.55 |
| 1:BH:341:THR:HG22 | 1:BH:343:THR:H | 1.71 | 0.55 |
| 1:BH:339:CYS:HB3 | 1:BH:348:PHE:CE2 | 2.42 | 0.55 |
| 1:BH:88:SER:O | 1:BH:91:GLN:N | 2.39 | 0.55 |
| 2:BJ:161:SER:O | 2:BJ:164:SER:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:20:GLN:HA | 2:BJ:70:ASP:HA | 1.87 | 0.55 |
| 2:BJ:708:ILE:HG13 | 2:BJ:727:PHE:CD2 | 2.41 | 0.55 |
| 4:CD:67:TYR:HD1 | 4:CD:84:ARG:HB3 | 1.70 | 0.55 |
| 5:CF:214:SER:OG | 5:CF:222:LEU:O | 2.22 | 0.55 |
| 6:CJ:23:LYS:HB3 | 6:CJ:26:ASP:HB2 | 1.88 | 0.55 |
| 3:D:231:TRP:O | 3:D:234:ASP:N | 2.39 | 0.55 |
| 5:CF:356:TYR:CE1 | 6:DA:4:LEU:HD13 | 2.41 | 0.55 |
| 7:DD:194:ALA:HB2 | 7:DD:208:TYR:HB3 | 1.88 | 0.55 |
| 12:DJ:111:ILE:O | 12:DJ:115:ASN:N | 2.28 | 0.55 |
| 1:EA:303:ASN:ND2 | 1:EA:310:PHE:CE2 | 2.74 | 0.55 |
| 1:EA:9:GLN:OE1 | 1:EA:9:GLN:N | 2.39 | 0.55 |
| 1:EB:400:ASN:OD1 | 1:EB:401:LEU:N | 2.39 | 0.55 |
| 2:EC:708:ILE:HG13 | 2:EC:727:PHE:CD2 | 2.41 | 0.55 |
| 2:EC:768:TYR:CG | 3:EE:197:ASP:HB3 | 2.41 | 0.55 |
| 4:EG:141:SER:HB3 | 4:EG:164:ILE:HD11 | 1.87 | 0.55 |
| 5:EI:213:GLY:O | 5:EI:214:SER:OG | 2.22 | 0.55 |
| 5:EJ:129:ARG:HG3 | 5:EJ:130:PHE:H | 1.70 | 0.55 |
| 5:EJ:202:TYR:HE1 | 5:EJ:206:PHE:HD1 | 1.54 | 0.55 |
| 5:FA:322:GLY:HA2 | 5:FA:360:THR:H | 1.72 | 0.55 |
| 7:FG:29:ILE:O | 7:FG:30:THR:OG1 | 2.19 | 0.55 |
| 8:FH:69:TRP:HZ3 | 8:FH:157:LEU:HD12 | 1.72 | 0.55 |
| 1:GE:346:ASP:HB2 | 1:GE:360:VAL:HG13 | 1.87 | 0.55 |
| 2:GF:125:GLU:HG2 | 2:GF:134:TYR:CD1 | 2.40 | 0.55 |
| 2:GF:138:ASN:OD1 | 2:GF:139:ASN:N | 2.40 | 0.55 |
| 2:GF:161:SER:O | 2:GF:164:SER:N | 2.39 | 0.55 |
| 2:GF:458:ASP:OD1 | 2:GF:472:LYS:HB2 | 2.06 | 0.55 |
| 3:GG:231:TRP:O | 3:GG:234:ASP:N | 2.39 | 0.55 |
| 3:GH:197:ASP:OD1 | 3:GH:197:ASP:N | 2.39 | 0.55 |
| 4:GJ:154:ASP:HB2 | 4:GJ:157:THR:HB | 1.88 | 0.55 |
| 4:HA:1:MET:HG2 | 4:HA:70:HIS:CE1 | 2.41 | 0.55 |
| 5:HB:371:PHE:CZ | 5:HB:373:SER:HB3 | 2.41 | 0.55 |
| 5:HB:63:GLU:HB2 | 5:HB:68:TYR:OH | 2.07 | 0.55 |
| 5:HC:191:ILE:H | 5:HD:164:ARG:HH21 | 1.55 | 0.55 |
| 5:HD:415:ASP:HB2 | 5:HD:440:GLN:HE22 | 1.71 | 0.55 |
| 5:HD:477:SER:N | 5:HD:602:ALA:O | 2.28 | 0.55 |
| 7:HH:144:ILE:HG21 | 7:HI:156:ASP:O | 2.06 | 0.55 |
| 7:HI:295:ILE:HG13 | 7:HJ:301:ARG:HB3 | 1.88 | 0.55 |
| 7:HI:447:HIS:HD2 | 7:HJ:447:HIS:CD2 | 2.23 | 0.55 |
| 7:HJ:392:LEU:HD22 | 7:HJ:523:ILE:HG21 | 1.88 | 0.55 |
| 12:IF:247:VAL:HG12 | 12:IF:248:MET:H | 1.71 | 0.55 |
| 5:J:271:THR:HB | 5:J:273:LYS:HG2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:407:TYR:HD2 | 5:J:407:TYR:CD2 | 2.23 | 0.55 |
| 6:L:23:LYS:HB3 | 6:L:26:ASP:HB2 | 1.89 | 0.55 |
| 7:O:399:PHE:HZ | 7:O:516:ASN:HD22 | 1.53 | 0.55 |
| 7:O:144:ILE:HG21 | 7:P:156:ASP:O | 2.05 | 0.55 |
| 7:O:14:ARG:NH2 | 7:P:19:ASP:OD2 | 2.40 | 0.55 |
| 7:Q:392:LEU:HD22 | 7:Q:523:ILE:HG21 | 1.89 | 0.55 |
| 10:U:209:TRP:HB2 | 10:U:223:ILE:HD12 | 12.87 | 0.55 |
| 10:U:58:TYR:HE1 | 12:IF:144:ASN:H | 1.53 | 0.55 |
| 1:Y:45:ASP:C | 1:Y:47:ASP:H | 2.10 | 0.55 |
| 13:YA:214[E]:MET:HG2 | 13:YA:232[E]:ASN:O | 2.06 | 0.55 |
| 13:YA:26[E]:ARG:HA | 13:YA:55[E]:MET:O | 2.05 | 0.55 |
| 13:YA:503[B]:THR:O | 13:YB:495[B]:THR:HA | 2.06 | 0.55 |
| 13:YB:498[D]:VAL:HA | 13:YC:490[D]:VAL:O | 2.07 | 0.55 |
| 13:YB:26[B]:ARG:HA | 13:YB:55[B]:MET:O | 2.06 | 0.55 |
| 13:YB:572[E]:ILE:HA | 13:YC:565[E]:TYR:O | 2.06 | 0.55 |
| 13:YB:61[F]:ILE:HA | 13:YC:76[F]:PRO:C | 2.27 | 0.55 |
| 13:YB:57[F]:VAL:CB | 13:YB:76[F]:PRO:HD3 | 2.37 | 0.55 |
| 1:EA:526:PRO:HB3 | 13:YC:254[C]:ARG:HD3 | 1.87 | 0.55 |
| 13:YC:88[B]:ASP:OD1 | 13:YC:88[B]:ASP:N | 2.38 | 0.55 |
| 14:YD:156[A]:TYR:O | 14:YD:177[A]:ALA:HA | 2.06 | 0.55 |
| 14:YD:301[D]:MET:HA | 14:YD:304[D]:TYR:HD2 | 1.71 | 0.55 |
| 14:YE:156[E]:TYR:O | 14:YE:177[E]:ALA:HA | 2.06 | 0.55 |
| 14:YE:178[B]:LEU:HD11 | 14:YE:183[B]:ASP:HA | 1.89 | 0.55 |
| 14:YE:292[C]:TYR:CD1 | 14:YE:371[C]:LYS:HB3 | 2.41 | 0.55 |
| 14:YE:301[B]:MET:HA | 14:YE:304[B]:TYR:HD2 | 1.71 | 0.55 |
| 14:YE:301[F]:MET:HA | 14:YE:304[F]:TYR:HD2 | 1.71 | 0.55 |
| 14:YF:156[B]:TYR:O | 14:YF:177[B]:ALA:HA | 2.07 | 0.55 |
| 14:YF:189[B]:TRP:NE1 | 14:YF:320[B]:PRO:HG2 | 2.21 | 0.55 |
| 2:Z:794:ASN:HB2 | 2:Z:814:HIS:CE1 | 2.42 | 0.55 |
| 1:A:339:CYS:HB3 | 1:A:348:PHE:CE2 | 2.42 | 0.55 |
| 1:A:582:ASN:OD1 | 1:A:585:GLY:N | 2.27 | 0.55 |
| 5:AC:407:TYR:HD2 | 5:AD:407:TYR:CD2 | 2.24 | 0.55 |
| 5:AD:304:ILE:HG13 | 5:AD:386:PHE:H | 1.72 | 0.55 |
| 6:AG:69:THR:HA | 6:AH:73:ASN:HB3 | 1.89 | 0.55 |
| 7:AJ:429:CYS:HG | 7:BA:515:TRP:HE1 | 1.54 | 0.55 |
| 1:BI:441:ILE:HD11 | 1:BI:644:ASN:ND2 | 2.21 | 0.55 |
| 2:BJ:422:GLU:HB3 | 2:BJ:423:GLU:OE1 | 2.06 | 0.55 |
| 2:BJ:738:LYS:HD2 | 2:BJ:882:PHE:O | 2.06 | 0.55 |
| 2:BJ:793:CYS:HB3 | 2:BJ:813:ILE:HG12 | 1.87 | 0.55 |
| 3:CB:29:GLY:HA3 | 3:CB:34:LYS:HB2 | 1.87 | 0.55 |
| 5:CG:271:THR:HB | 5:CG:273:LYS:HG2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:285:LEU:CD1 | 5:CH:375:PHE:HB2 | 2.36 | 0.55 |
| 6:CI:192:THR:HB | 6:CI:219:ALA:HB3 | 1.87 | 0.55 |
| 3:D:195:PRO:HG3 | 3:D:222:ARG:HD3 | 1.89 | 0.55 |
| 7:DB:301:ARG:HB3 | 7:DD:295:ILE:HG13 | 1.87 | 0.55 |
| 7:DB:497:ASN:H | 7:DB:500:TYR:HB2 | 1.71 | 0.55 |
| 7:DC:99:ARG:NH1 | 7:DC:101:SER:HB3 | 2.22 | 0.55 |
| 11:DI:17:ASN:ND2 | 11:DI:19:ASN:O | 2.39 | 0.55 |
| 3:E:96:GLY:HA2 | 3:E:104:TYR:CE1 | 2.40 | 0.55 |
| 1:EA:388:GLN:O | 1:EA:392:ILE:HG22 | 2.06 | 0.55 |
| 1:EA:448:TYR:CZ | 1:EA:642:PHE:HB2 | 2.41 | 0.55 |
| 1:EB:441:ILE:HD11 | 1:EB:644:ASN:ND2 | 2.21 | 0.55 |
| 2:EC:138:ASN:OD1 | 2:EC:139:ASN:N | 2.40 | 0.55 |
| 2:EC:825:GLU:N | 2:EC:837:GLU:OE1 | 2.40 | 0.55 |
| 2:EC:969:TYR:O | 2:EC:973:ASN:N | 2.29 | 0.55 |
| 4:EG:1:MET:HG2 | 4:EG:70:HIS:CE1 | 2.42 | 0.55 |
| 4:EF:39:TYR:CD1 | 4:EG:7:LYS:HB2 | 2.42 | 0.55 |
| 5:EI:358:VAL:HA | 5:EI:371:PHE:HA | 1.86 | 0.55 |
| 5:EI:419:ASP:HB3 | 5:EI:436:VAL:HB | 1.88 | 0.55 |
| 5:EJ:271:THR:HB | 5:EJ:273:LYS:HG2 | 1.89 | 0.55 |
| 5:EJ:361:ASP:HB3 | 5:EJ:362:GLU:OE1 | 2.06 | 0.55 |
| 4:F:154:ASP:HB2 | 4:F:157:THR:HB | 1.88 | 0.55 |
| 4:F:275:ALA:O | 4:G:282:GLN:NE2 | 2.39 | 0.55 |
| 5:FA:212:PHE:CZ | 5:FA:230:ILE:HB | 2.41 | 0.55 |
| 7:FF:211:SER:H | 7:FF:214:THR:HG1 | 1.48 | 0.55 |
| 7:FF:236:VAL:HG21 | 7:FF:249:THR:HB | 1.88 | 0.55 |
| 7:FF:99:ARG:NH1 | 7:FF:101:SER:HB3 | 2.22 | 0.55 |
| 8:FH:14:ASP:OD2 | 8:FH:17:ARG:NH2 | 2.33 | 0.55 |
| 1:GD:145:PHE:CZ | 1:GD:286:PHE:HE1 | 2.24 | 0.55 |
| 3:GG:263:LEU:HB2 | 3:GG:266:ASN:HB2 | 1.89 | 0.55 |
| 2:EC:509:TYR:HB2 | 3:GH:175:ASP:OD2 | 2.07 | 0.55 |
| 4:GI:67:TYR:HD1 | 4:GI:84:ARG:HB3 | 1.70 | 0.55 |
| 4:H:1:MET:HG2 | 4:H:70:HIS:CE1 | 2.41 | 0.55 |
| 5:HB:407:TYR:HD2 | 5:HC:407:TYR:CD2 | 2.24 | 0.55 |
| 5:HB:60:LEU:HG | 5:HB:79:ILE:HG22 | 1.87 | 0.55 |
| 5:HC:65:GLY:O | 5:HD:45:SER:OG | 2.13 | 0.55 |
| 7:HH:40:SER:HB3 | 7:HI:24:ASN:HB3 | 1.88 | 0.55 |
| 5:I:358:VAL:HG22 | 5:I:371:PHE:HB2 | 1.88 | 0.55 |
| 5:J:317:LEU:HD13 | 5:K:312:ARG:NH2 | 2.21 | 0.55 |
| 5:K:285:LEU:CD1 | 5:K:375:PHE:HB2 | 2.36 | 0.55 |
| 7:Q:29:ILE:O | 7:Q:30:THR:OG1 | 2.19 | 0.55 |
| 8:S:69:TRP:HZ3 | 8:S:157:LEU:HD12 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:S:55:ASN:HB3 | 8:BC:99:ILE:HD11 | 1.88 | 0.55 |
| 13:YA:214[A]:MET:HG2 | 13:YA:232[A]:ASN:O | 2.06 | 0.55 |
| 13:YA:88[F]:ASP:N | 13:YA:88[F]:ASP:OD1 | 2.38 | 0.55 |
| 13:YA:89[C]:LYS:O | 13:YA:91[C]:LYS:HG3 | 2.06 | 0.55 |
| 13:YB:25[F]:GLY:HA3 | 13:YB:73[F]:VAL:HG12 | 1.87 | 0.55 |
| 13:YA:527[C]:THR:O | 13:YB:519[C]:THR:HA | 2.05 | 0.55 |
| 13:YB:321[F]:LYS:HG2 | 13:YC:453[F]:ASP:OD1 | 2.05 | 0.55 |
| 14:YD:292[E]:TYR:CD1 | 14:YD:371[E]:LYS:HB3 | 2.41 | 0.55 |
| 14:YD:292[D]:TYR:CD1 | 14:YD:371[D]:LYS:HB3 | 2.41 | 0.55 |
| 14:YE:156[F]:TYR:O | 14:YE:177[F]:ALA:HA | 2.06 | 0.55 |
| 14:YF:301[F]:MET:HA | 14:YF:304[F]:TYR:HD2 | 1.71 | 0.55 |
| 14:YF:189[C]:TRP:NE1 | 14:YF:320[C]:PRO:HG2 | 2.21 | 0.55 |
| 2:Z:708:ILE:HG13 | 2:Z:727:PHE:CD2 | 2.41 | 0.55 |
| 5:AD:290:SER:HA | 5:AD:371:PHE:HB3 | 1.88 | 0.55 |
| 5:AE:289:LYS:HE2 | 5:AE:370:HIS:CE1 | 2.42 | 0.55 |
| 7:AI:12:GLU:HG3 | 7:AI:14:ARG:H | 1.71 | 0.55 |
| 7:AI:289:GLN:OE1 | 7:AI:294:GLN:NE2 | 2.40 | 0.55 |
| 11:BF:133:TRP:CZ2 | 11:BF:150:LEU:HD11 | 2.42 | 0.55 |
| 1:BH:388:GLN:O | 1:BH:392:ILE:HG22 | 2.07 | 0.55 |
| 1:BI:213:SER:OG | 1:BI:337:GLN:OE1 | 2.23 | 0.55 |
| 1:BI:455:PHE:HD2 | 1:BI:456:ASN:HB2 | 1.72 | 0.55 |
| 2:BJ:138:ASN:OD1 | 2:BJ:139:ASN:N | 2.40 | 0.55 |
| 2:BJ:768:TYR:CG | 3:CB:197:ASP:HB3 | 2.41 | 0.55 |
| 2:C:738:LYS:HD2 | 2:C:882:PHE:O | 2.06 | 0.55 |
| 2:C:964:PRO:HG2 | 2:C:966:PRO:HG3 | 1.89 | 0.55 |
| 3:CA:195:PRO:HG3 | 3:CA:222:ARG:HD3 | 1.89 | 0.55 |
| 4:CC:69:LYS:NZ | 4:CD:103:LEU:O | 2.29 | 0.55 |
| 4:CC:7:LYS:NZ | 4:CE:36:ASN:OD1 | 2.27 | 0.55 |
| 5:CF:371:PHE:CZ | 5:CF:373:SER:HB3 | 2.41 | 0.55 |
| 5:CG:202:TYR:HE1 | 5:CG:206:PHE:HD1 | 1.54 | 0.55 |
| 5:CG:312:ARG:O | 5:CG:382:ASN:N | 2.30 | 0.55 |
| 5:CG:361:ASP:HB3 | 5:CG:362:GLU:OE1 | 2.06 | 0.55 |
| 5:CG:290:SER:HA | 5:CG:371:PHE:HB3 | 1.88 | 0.55 |
| 5:CH:316:ILE:HG21 | 6:CJ:7:LYS:HG3 | 1.89 | 0.55 |
| 3:D:130:VAL:HG12 | 3:D:191:LEU:HD12 | 1.87 | 0.55 |
| 8:DF:69:TRP:HZ3 | 8:DF:157:LEU:HD12 | 1.72 | 0.55 |
| 1:EA:212:LYS:HA | 1:EA:399:TYR:OH | 2.05 | 0.55 |
| 1:EB:279:ASP:OD1 | 1:EB:280:ALA:N | 2.39 | 0.55 |
| 1:EB:346:ASP:HB2 | 1:EB:360:VAL:HG13 | 1.87 | 0.55 |
| 1:EB:70:PHE:HE2 | 2:EC:686:LEU:CB | 2.17 | 0.55 |
| 3:ED:231:TRP:O | 3:ED:234:ASP:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:EE:197:ASP:OD1 | 3:EE:197:ASP:N | 2.38 | 0.55 |
| 5:EI:339:GLU:HB3 | 6:FC:172:SER:O | 2.06 | 0.55 |
| 5:EJ:304:ILE:HG13 | 5:EJ:386:PHE:H | 1.72 | 0.55 |
| 8:FI:69:TRP:HZ3 | 8:FI:157:LEU:HD12 | 1.72 | 0.55 |
| 12:GC:165:ASP:OD1 | 12:GC:166:SER:N | 2.40 | 0.55 |
| 1:GD:8:TYR:CZ | 1:GD:20:ILE:HG22 | 2.42 | 0.55 |
| 2:GF:450:PHE:CZ | 2:GF:473:TYR:CE1 | 2.94 | 0.55 |
| 2:GF:712:ASN:HD21 | 2:GF:720:ARG:HG3 | 1.70 | 0.55 |
| 2:GF:825:GLU:N | 2:GF:837:GLU:OE1 | 2.40 | 0.55 |
| 4:GI:154:ASP:HB2 | 4:GI:157:THR:HB | 1.88 | 0.55 |
| 5:HD:262:GLN:HA | 5:HD:381:ILE:O | 2.06 | 0.55 |
| 7:HI:99:ARG:NH1 | 7:HI:101:SER:HB3 | 2.22 | 0.55 |
| 7:HI:310:ASN:OD1 | 7:HI:311:GLY:N | 2.39 | 0.55 |
| 5:HD:196:ARG:NE | 7:HI:5:THR:HG23 | 2.22 | 0.55 |
| 5:I:196:ARG:HH11 | 7:O:5:THR:HG23 | 1.71 | 0.55 |
| 5:I:535:THR:O | 5:K:576:THR:N | 2.31 | 0.55 |
| 8:IB:69:TRP:HZ3 | 8:IB:157:LEU:HD12 | 1.72 | 0.55 |
| 5:J:490:TRP:NE1 | 5:J:515:THR:O | 2.40 | 0.55 |
| 5:K:262:GLN:HA | 5:K:381:ILE:O | 2.05 | 0.55 |
| 7:Q:386:ASN:OD1 | 7:Q:389:ASN:N | 2.24 | 0.55 |
| 7:O:439:ILE:HG23 | 7:Q:515:TRP:CH2 | 2.40 | 0.55 |
| 8:S:34:PHE:HD2 | 8:IB:9:ALA:HB2 | 1.71 | 0.55 |
| 12:W:217:THR:O | 12:W:246:ARG:N | 2.32 | 0.55 |
| 1:X:341:THR:HG22 | 1:X:343:THR:H | 1.71 | 0.55 |
| 13:YA:265[E]:VAL:HG22 | 13:YA:300[E]:LEU:HD23 | 1.88 | 0.55 |
| 13:YA:25[B]:GLY:HA3 | 13:YA:73[B]:VAL:HG12 | 1.87 | 0.55 |
| 13:YB:214[A]:MET:HG2 | 13:YB:232[A]:ASN:O | 2.06 | 0.55 |
| 13:YB:284[C]:MET:HE3 | 13:YC:363[C]:PRO:CB | 2.36 | 0.55 |
| 13:YB:89[A]:LYS:O | 13:YB:91[A]:LYS:HG3 | 2.06 | 0.55 |
| 13:YC:265[A]:VAL:HG22 | 13:YC:300[A]:LEU:HD23 | 1.88 | 0.55 |
| 13:YC:26[B]:ARG:HA | 13:YC:55[B]:MET:O | 2.06 | 0.55 |
| 13:YA:534[F]:LEU:HD22 | 13:YC:538[F]:VAL:HG21 | 1.89 | 0.55 |
| 13:YB:572[B]:ILE:HA | 13:YC:565[B]:TYR:O | 2.06 | 0.55 |
| 13:YC:57[F]:VAL:CB | 13:YC:76[F]:PRO:HD3 | 2.37 | 0.55 |
| 14:YD:156[B]:TYR:O | 14:YD:177[B]:ALA:HA | 2.07 | 0.55 |
| 14:YD:245[B]:ARG:HD3 | 14:YD:305[B]:ASP:OD2 | 2.06 | 0.55 |
| 14:YD:245[C]:ARG:HD3 | 14:YD:305[C]:ASP:OD2 | 2.06 | 0.55 |
| 14:YD:189[F]:TRP:NE1 | 14:YD:320[F]:PRO:HG2 | 2.21 | 0.55 |
| 14:YF:156[C]:TYR:O | 14:YF:177[C]:ALA:HA | 2.07 | 0.55 |
| 14:YF:178[F]:LEU:HD11 | 14:YF:183[F]:ASP:HA | 1.89 | 0.55 |
| 14:YF:64[F]:MET:HE3 | 14:YF:68[F]:GLU:HG3 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:98[F]:ASP:OD1 | 14:YF:99[F]:SER:N | 2.38 | 0.55 |
| 2:Z:189:ARG:HG2 | 2:Z:204:ARG:NH1 | 2.22 | 0.55 |
| 2:Z:20:GLN:HA | 2:Z:70:ASP:HA | 1.87 | 0.55 |
| 1:A:88:SER:O | 1:A:91:GLN:N | 2.39 | 0.55 |
| 4:AA:1:MET:HG2 | 4:AA:70:HIS:CE1 | 2.41 | 0.55 |
| 5:AC:501:LEU:HD13 | 5:AC:512:PRO:HG2 | 1.88 | 0.55 |
| 5:AD:490:TRP:NE1 | 5:AD:515:THR:O | 2.40 | 0.55 |
| 5:AE:272:SER:OG | 6:AH:106:THR:N | 2.26 | 0.55 |
| 5:AE:322:GLY:HA2 | 5:AE:360:THR:H | 1.72 | 0.55 |
| 7:AI:406:GLY:O | 7:AI:410:THR:HG23 | 2.06 | 0.55 |
| 1:BH:209:TRP:HB2 | 1:BH:223:ILE:HD12 | 1.89 | 0.55 |
| 1:BH:145:PHE:CZ | 1:BH:286:PHE:HE1 | 2.24 | 0.55 |
| 1:BI:400:ASN:OD1 | 1:BI:401:LEU:N | 2.39 | 0.55 |
| 1:BI:544:ASP:CB | 1:BI:576:ASP:HB2 | 2.36 | 0.55 |
| 2:BJ:458:ASP:OD1 | 2:BJ:472:LYS:HB2 | 2.05 | 0.55 |
| 2:BJ:504:GLN:CD | 2:BJ:505:PRO:HD2 | 2.27 | 0.55 |
| 2:C:319:TYR:HD1 | 2:C:328:TYR:HB2 | 1.71 | 0.55 |
| 2:C:351:GLU:CB | 2:C:353:ASP:HB2 | 2.31 | 0.55 |
| 4:CD:202:LEU:HA | 4:CD:278:VAL:HA | 1.87 | 0.55 |
| 5:CG:258:TYR:O | 5:CG:259:THR:OG1 | 2.24 | 0.55 |
| 7:DB:297:TYR:HB2 | 7:DD:291:ARG:HA | 1.87 | 0.55 |
| 7:DB:339:ARG:CZ | 7:DD:358:ALA:HB2 | 2.37 | 0.55 |
| 11:DI:133:TRP:CZ2 | 11:DI:150:LEU:HD11 | 2.42 | 0.55 |
| 2:EC:161:SER:O | 2:EC:164:SER:N | 2.39 | 0.55 |
| 2:EC:653:MET:HB3 | 2:EC:658:LEU:HD11 | 1.89 | 0.55 |
| 4:EF:53:GLY:HA3 | 4:EG:7:LYS:HE2 | 1.89 | 0.55 |
| 4:F:218:GLU:OE1 | 4:G:201:LYS:NZ | 2.31 | 0.55 |
| 5:FA:18:TYR:HB2 | 5:FA:21:LYS:H | 1.71 | 0.55 |
| 7:FG:383:TYR:CD1 | 7:FG:393:PRO:HG3 | 2.41 | 0.55 |
| 8:DE:117:ALA:HA | 8:FH:77:GLU:OE2 | 2.07 | 0.55 |
| 12:GC:126:TYR:HA | 12:IF:230:TYR:CD2 | 2.41 | 0.55 |
| 3:GG:114:CYS:HA | 3:GG:120:ASN:OD1 | 2.05 | 0.55 |
| 5:HC:202:TYR:HE1 | 5:HC:206:PHE:HD1 | 1.54 | 0.55 |
| 5:I:372:ASP:N | 5:I:372:ASP:OD1 | 2.40 | 0.55 |
| 10:ID:129:LEU:HD13 | 10:ID:209:TRP:HZ3 | 1.70 | 0.55 |
| 5:J:36:GLU:HA | 5:J:50:LYS:NZ | 2.22 | 0.55 |
| 5:K:357:SER:OG | 6:M:4:LEU:HD21 | 2.06 | 0.55 |
| 7:O:233:GLN:HG3 | 5:HB:348:THR:H | 1.72 | 0.55 |
| 7:O:289:GLN:OE1 | 7:O:294:GLN:NE2 | 2.39 | 0.55 |
| 8:R:14:ASP:OD2 | 8:R:17:ARG:NH2 | 2.33 | 0.55 |
| 11:V:142:LYS:HB3 | 11:V:143:TYR:HD2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:W:218:MET:SD | 12:W:243:PHE:CD2 | 2.99 | 0.55 |
| 1:X:212:LYS:HA | 1:X:399:TYR:OH | 2.05 | 0.55 |
| 1:X:448:TYR:CZ | 1:X:642:PHE:HB2 | 2.41 | 0.55 |
| 1:Y:544:ASP:CB | 1:Y:576:ASP:HB2 | 2.36 | 0.55 |
| 13:YA:193[E]:ASP:OD1 | 13:YA:197[E]:TYR:N | 2.33 | 0.55 |
| 13:YA:293[B]:ASN:O | 13:YA:297[B]:THR:N | 2.40 | 0.55 |
| 13:YA:293[C]:ASN:O | 13:YA:297[C]:THR:N | 2.39 | 0.55 |
| 13:YA:425[C]:SER:HB2 | 13:YA:426[C]:PRO:HD2 | 1.89 | 0.55 |
| 13:YA:425[E]:SER:HB2 | 13:YA:426[E]:PRO:HD2 | 1.89 | 0.55 |
| 13:YB:425[C]:SER:HB2 | 13:YB:426[C]:PRO:HD2 | 1.89 | 0.55 |
| 13:YB:47[A]:ILE:HG23 | 14:YE:123[A]:PRO:CG | 2.31 | 0.55 |
| 13:YA:503[A]:THR:O | 13:YB:495[A]:THR:HA | 2.06 | 0.55 |
| 13:YB:572[C]:ILE:HA | 13:YC:565[C]:TYR:O | 2.06 | 0.55 |
| 13:YB:61[B]:ILE:HA | 13:YC:76[B]:PRO:C | 2.27 | 0.55 |
| 13:YB:61[B]:ILE:HG23 | 13:YC:60[B]:PRO:HD3 | 1.88 | 0.55 |
| 13:YC:193[A]:ASP:OD1 | 13:YC:197[A]:TYR:N | 2.33 | 0.55 |
| 14:YD:156[D]:TYR:O | 14:YD:177[D]:ALA:HA | 2.06 | 0.55 |
| 14:YD:189[D]:TRP:NE1 | 14:YD:320[D]:PRO:HG2 | 2.21 | 0.55 |
| 14:YD:64[D]:MET:HE3 | 14:YD:68[D]:GLU:HG3 | 1.87 | 0.55 |
| 14:YE:292[B]:TYR:CD1 | 14:YE:371[B]:LYS:HB3 | 2.41 | 0.55 |
| 14:YE:245[A]:ARG:HD3 | 14:YE:305[A]:ASP:OD2 | 2.06 | 0.55 |
| 14:YF:156[D]:TYR:O | 14:YF:177[D]:ALA:HA | 2.07 | 0.55 |
| 14:YF:156[F]:TYR:O | 14:YF:177[F]:ALA:HA | 2.06 | 0.55 |
| 11:DI:190:LYS:HE3 | 14:YF:24[A]:SER:O | 2.05 | 0.55 |
| 14:YF:292[A]:TYR:CD1 | 14:YF:371[A]:LYS:HB3 | 2.41 | 0.55 |
| 2:Z:433:ASN:O | 2:Z:443:LEU:HA | 2.06 | 0.55 |
| 2:Z:794:ASN:HB2 | 2:Z:814:HIS:NE2 | 2.22 | 0.55 |
| 1:A:209:TRP:HB2 | 1:A:223:ILE:HD12 | 1.89 | 0.55 |
| 1:A:341:THR:HG22 | 1:A:343:THR:H | 1.71 | 0.55 |
| 1:A:9:GLN:N | 1:A:9:GLN:OE1 | 2.39 | 0.55 |
| 5:AD:9:ASN:OD1 | 5:AD:10:VAL:N | 2.39 | 0.55 |
| 5:AD:358:VAL:HG22 | 5:AD:371:PHE:HB2 | 1.89 | 0.55 |
| 7:AI:513:ARG:O | 7:AJ:441:GLN:N | 2.30 | 0.55 |
| 7:AI:130:GLU:HA | 7:AJ:139:ASN:HD21 | 1.72 | 0.55 |
| 7:AI:144:ILE:HG21 | 7:AJ:156:ASP:O | 2.05 | 0.55 |
| 8:BC:69:TRP:HZ3 | 8:BC:157:LEU:HD12 | 1.72 | 0.55 |
| 12:BG:165:ASP:OD1 | 12:BG:166:SER:N | 2.40 | 0.55 |
| 1:BI:346:ASP:HB2 | 1:BI:360:VAL:HG13 | 1.87 | 0.55 |
| 2:BJ:437:ASP:HA | 2:BJ:516:TRP:CE3 | 2.42 | 0.55 |
| 2:BJ:450:PHE:CZ | 2:BJ:473:TYR:CE1 | 2.94 | 0.55 |
| 2:C:184:CYS:O | 2:C:185:LYS:HG2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:189:ARG:HG2 | 2:C:204:ARG:NH1 | 2.22 | 0.55 |
| 3:CA:313:GLU:HG3 | 3:CB:10:ALA:HB2 | 1.89 | 0.55 |
| 4:CC:154:ASP:HB2 | 4:CC:157:THR:HB | 1.88 | 0.55 |
| 5:CF:175:THR:O | 5:CF:232:LEU:N | 2.35 | 0.55 |
| 5:CG:36:GLU:HA | 5:CG:50:LYS:NZ | 2.22 | 0.55 |
| 5:CF:407:TYR:HD2 | 5:CG:407:TYR:CD2 | 2.25 | 0.55 |
| 5:CG:490:TRP:NE1 | 5:CG:515:THR:O | 2.40 | 0.55 |
| 5:CG:326:MET:HE1 | 5:CH:264:ARG:H | 1.71 | 0.55 |
| 5:CH:264:ARG:HG3 | 5:CH:379:ASP:O | 2.07 | 0.55 |
| 5:CG:317:LEU:HD13 | 5:CH:312:ARG:NH2 | 2.22 | 0.55 |
| 5:CH:31:ASP:O | 5:CH:35:TYR:N | 2.27 | 0.55 |
| 7:DC:29:ILE:O | 7:DC:30:THR:OG1 | 2.24 | 0.55 |
| 7:DC:93:THR:HG22 | 7:DC:94:VAL:HG23 | 1.88 | 0.55 |
| 7:DD:20:PRO:HG3 | 7:DD:29:ILE:HG13 | 1.89 | 0.55 |
| 3:E:197:ASP:N | 3:E:197:ASP:OD1 | 2.38 | 0.55 |
| 1:EB:90:VAL:HG13 | 1:EB:100:PRO:HG3 | 1.87 | 0.55 |
| 1:EB:76:TYR:HB3 | 1:EB:82:THR:HG21 | 1.87 | 0.55 |
| 2:EC:184:CYS:O | 2:EC:185:LYS:HG2 | 2.07 | 0.55 |
| 2:EC:20:GLN:HA | 2:EC:70:ASP:HA | 1.87 | 0.55 |
| 2:EC:251:ASP:O | 2:EC:301:PRO:HG2 | 2.06 | 0.55 |
| 2:EC:437:ASP:HA | 2:EC:516:TRP:CE3 | 2.42 | 0.55 |
| 2:EC:738:LYS:HD2 | 2:EC:882:PHE:O | 2.06 | 0.55 |
| 3:ED:195:PRO:HG3 | 3:ED:222:ARG:HD3 | 1.89 | 0.55 |
| 5:EI:63:GLU:HB2 | 5:EI:68:TYR:OH | 2.07 | 0.55 |
| 5:EJ:318:GLN:HE22 | 6:FB:8:ALA:N | 2.05 | 0.55 |
| 5:EJ:358:VAL:HG22 | 5:EJ:371:PHE:HB2 | 1.89 | 0.55 |
| 7:FE:497:ASN:H | 7:FE:500:TYR:HB2 | 1.71 | 0.55 |
| 7:FE:112:ASN:HA | 7:FG:117:THR:OG1 | 2.07 | 0.55 |
| 1:GD:209:TRP:HB2 | 1:GD:223:ILE:HD12 | 1.89 | 0.55 |
| 1:GD:388:GLN:O | 1:GD:392:ILE:HG22 | 2.06 | 0.55 |
| 2:GF:433:ASN:O | 2:GF:443:LEU:HA | 2.06 | 0.55 |
| 4:GI:172:GLU:HA | 4:GJ:166:SER:H | 1.71 | 0.55 |
| 4:GJ:172:GLU:HA | 4:HA:166:SER:H | 1.71 | 0.55 |
| 4:GJ:67:TYR:HD1 | 4:GJ:84:ARG:HB3 | 1.70 | 0.55 |
| 4:GI:7:LYS:NZ | 4:HA:36:ASN:OD1 | 2.24 | 0.55 |
| 7:HH:438:GLN:HB2 | 7:HJ:516:ASN:OD1 | 2.06 | 0.55 |
| 5:HB:196:ARG:HH11 | 7:HH:5:THR:HG23 | 1.72 | 0.55 |
| 7:HH:130:GLU:HA | 7:HI:139:ASN:HD21 | 1.72 | 0.55 |
| 5:I:214:SER:OG | 5:I:222:LEU:O | 2.22 | 0.55 |
| 5:I:63:GLU:HB2 | 5:I:68:TYR:OH | 2.07 | 0.55 |
| 11:IE:17:ASN:ND2 | 11:IE:19:ASN:O | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:256:SER:HB2 | 5:J:387:ASN:OD1 | 2.06 | 0.55 |
| 5:K:506:LEU:HB3 | 5:K:510:GLY:HA2 | 1.89 | 0.55 |
| 6:M:23:LYS:HB3 | 6:M:26:ASP:HB2 | 1.88 | 0.55 |
| 6:N:23:LYS:HB3 | 6:N:26:ASP:HB2 | 1.89 | 0.55 |
| 7:P:118:PRO:O | 7:P:122:THR:N | 2.36 | 0.55 |
| 7:P:463:THR:HG21 | 7:Q:490:ILE:HD12 | 1.88 | 0.55 |
| 7:Q:330:ARG:NH2 | 7:Q:336:GLU:OE2 | 2.39 | 0.55 |
| 7:O:339:ARG:CZ | 7:Q:358:ALA:HB2 | 2.37 | 0.55 |
| 7:O:441:GLN:N | 7:Q:513:ARG:O | 2.33 | 0.55 |
| 8:R:69:TRP:HZ3 | 8:R:157:LEU:HD12 | 1.72 | 0.55 |
| 11:V:17:ASN:ND2 | 11:V:19:ASN:O | 2.39 | 0.55 |
| 1:X:209:TRP:HB2 | 1:X:223:ILE:HD12 | 1.89 | 0.55 |
| 1:X:303:ASN:ND2 | 1:X:310:PHE:CE2 | 2.74 | 0.55 |
| 1:X:403:PRO:HG3 | 1:Y:404:ILE:HD12 | 1.89 | 0.55 |
| 1:Y:196:GLN:HG3 | 1:Y:273:ILE:HD12 | 1.88 | 0.55 |
| 13:YB:565[B]:TYR:CZ | 13:YC:557[B]:MET:HG2 | 2.42 | 0.55 |
| 13:YB:565[E]:TYR:CZ | 13:YC:557[E]:MET:HG2 | 2.42 | 0.55 |
| 13:YC:293[D]:ASN:O | 13:YC:297[D]:THR:N | 2.40 | 0.55 |
| 13:YC:425[E]:SER:HB2 | 13:YC:426[E]:PRO:HD2 | 1.89 | 0.55 |
| 14:YD:189[C]:TRP:NE1 | 14:YD:320[C]:PRO:HG2 | 2.21 | 0.55 |
| 14:YD:245[E]:ARG:HD3 | 14:YD:305[E]:ASP:OD2 | 2.06 | 0.55 |
| 14:YD:245[F]:ARG:HD3 | 14:YD:305[F]:ASP:OD2 | 2.06 | 0.55 |
| 14:YD:64[E]:MET:HE3 | 14:YD:68[E]:GLU:HG3 | 1.87 | 0.55 |
| 14:YE:64[C]:MET:HE3 | 14:YE:68[C]:GLU:HG3 | 1.87 | 0.55 |
| 14:YE:98[C]:ASP:OD1 | 14:YE:99[C]:SER:N | 2.39 | 0.55 |
| 14:YF:245[E]:ARG:HD3 | 14:YF:305[E]:ASP:OD2 | 2.06 | 0.55 |
| 2:Z:125:GLU:HG2 | 2:Z:134:TYR:CG | 2.41 | 0.55 |
| 2:Z:934:ALA:HB3 | 2:Z:997:SER:HB3 | 1.89 | 0.55 |
| 5:AC:293:PHE:HD1 | 5:AC:298:LEU:HD11 | 1.71 | 0.55 |
| 5:AC:156:SER:HB3 | 5:AD:154:ILE:HG12 | 1.87 | 0.55 |
| 1:BI:396:LEU:O | 1:BI:399:TYR:N | 2.40 | 0.55 |
| 2:BJ:146:LEU:HD13 | 2:BJ:582:ALA:HB1 | 1.87 | 0.55 |
| 2:BJ:251:ASP:O | 2:BJ:301:PRO:HG2 | 2.06 | 0.55 |
| 2:C:433:ASN:O | 2:C:443:LEU:HA | 2.06 | 0.55 |
| 2:C:450:PHE:CZ | 2:C:473:TYR:CE1 | 2.94 | 0.55 |
| 2:C:653:MET:HB3 | 2:C:658:LEU:HD11 | 1.89 | 0.55 |
| 2:C:934:ALA:HB3 | 2:C:997:SER:HB3 | 1.89 | 0.55 |
| 4:CC:53:GLY:HA3 | 4:CD:7:LYS:HE2 | 1.89 | 0.55 |
| 4:CC:7:LYS:HD3 | 4:CE:39:TYR:CG | 2.41 | 0.55 |
| 5:CF:186:TYR:OH | 5:CF:190:ASN:O | 2.19 | 0.55 |
| 5:CH:322:GLY:HA2 | 5:CH:360:THR:H | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:507:ASP:OD1 | 5:CH:511:ASN:N | 2.25 | 0.55 |
| 5:CH:339:GLU:HG2 | 6:CI:173:THR:HB | 1.87 | 0.55 |
| 7:DD:9:VAL:HG23 | 7:DD:10:SER:N | 2.20 | 0.55 |
| 7:DC:359:TRP:NE1 | 7:DD:340:THR:O | 2.36 | 0.55 |
| 1:EA:209:TRP:HB2 | 1:EA:223:ILE:HD12 | 1.89 | 0.55 |
| 1:EA:8:TYR:CZ | 1:EA:20:ILE:HG22 | 2.42 | 0.55 |
| 1:EB:189:ASP:HA | 11:GB:121:TYR:HE2 | 1.72 | 0.55 |
| 3:ED:263:LEU:HB2 | 3:ED:266:ASN:HB2 | 1.89 | 0.55 |
| 3:ED:313:GLU:HG3 | 3:EE:10:ALA:HB2 | 1.89 | 0.55 |
| 5:EJ:326:MET:HE1 | 5:FA:264:ARG:H | 1.72 | 0.55 |
| 7:FE:289:GLN:OE1 | 7:FE:294:GLN:NE2 | 2.40 | 0.55 |
| 7:FE:473:LYS:HB3 | 7:FF:473:LYS:HD2 | 1.89 | 0.55 |
| 7:FE:144:ILE:HG21 | 7:FF:156:ASP:O | 2.07 | 0.55 |
| 7:FG:20:PRO:HG3 | 7:FG:29:ILE:HG13 | 1.89 | 0.55 |
| 7:FG:255:SER:HB3 | 7:FG:263:VAL:HG13 | 1.89 | 0.55 |
| 11:GB:17:ASN:ND2 | 11:GB:19:ASN:O | 2.39 | 0.55 |
| 1:GD:246:ASN:ND2 | 1:GD:255:ASN:OD1 | 2.39 | 0.55 |
| 1:GE:400:ASN:OD1 | 1:GE:401:LEU:N | 2.39 | 0.55 |
| 5:HB:154:ILE:HB | 5:HD:156:SER:HB2 | 1.89 | 0.55 |
| 5:HC:9:ASN:OD1 | 5:HC:10:VAL:N | 2.39 | 0.55 |
| 5:HC:271:THR:HB | 5:HC:273:LYS:HG2 | 1.89 | 0.55 |
| 5:HB:36:GLU:HG3 | 5:HC:43:PRO:HG2 | 1.87 | 0.55 |
| 5:HC:490:TRP:NE1 | 5:HC:515:THR:O | 2.40 | 0.55 |
| 5:HD:506:LEU:HB3 | 5:HD:510:GLY:HA2 | 1.89 | 0.55 |
| 5:HC:318:GLN:HB3 | 6:HE:4:LEU:HG | 1.89 | 0.55 |
| 6:HF:100:PRO:O | 6:HF:103:SER:OG | 2.18 | 0.55 |
| 6:HG:23:LYS:HB3 | 6:HG:26:ASP:HB2 | 1.89 | 0.55 |
| 7:HH:146:SER:O | 7:HH:150:ALA:N | 2.38 | 0.55 |
| 7:HH:325:TYR:HD1 | 7:HH:330:ARG:HA | 1.72 | 0.55 |
| 7:HH:77:THR:HG23 | 7:HH:79:ALA:N | 2.22 | 0.55 |
| 5:I:146:VAL:HG21 | 5:J:153:LYS:HD3 | 1.89 | 0.55 |
| 5:I:371:PHE:CZ | 5:I:373:SER:HB3 | 2.41 | 0.55 |
| 8:IA:69:TRP:HZ3 | 8:IA:157:LEU:HD12 | 1.72 | 0.55 |
| 12:IF:222:SER:O | 12:IF:242:THR:N | 2.39 | 0.55 |
| 5:K:212:PHE:CZ | 5:K:230:ILE:HB | 2.41 | 0.55 |
| 7:O:40:SER:HB3 | 7:P:24:ASN:HB3 | 1.88 | 0.55 |
| 7:P:418:ASP:OD1 | 7:P:422:LYS:N | 2.38 | 0.55 |
| 10:U:129:LEU:HD13 | 10:U:209:TRP:HZ3 | 1.70 | 0.55 |
| 1:Y:441:ILE:HD11 | 1:Y:644:ASN:ND2 | 2.21 | 0.55 |
| 13:YA:293[F]:ASN:O | 13:YA:297[F]:THR:N | 2.39 | 0.55 |
| 13:YA:503[C]:THR:O | 13:YB:495[C]:THR:HA | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:534[B]:LEU:HD22 | 13:YC:538[B]:VAL:HG21 | 1.89 | 0.55 |
| 13:YA:87[E]:LEU:HD21 | 13:YA:95[E]:ILE:HG23 | 1.87 | 0.55 |
| 13:YA:442[D]:THR:HG21 | 13:YB:438[D]:LEU:HD22 | 1.89 | 0.55 |
| 13:YB:498[E]:VAL:HA | 13:YC:490[E]:VAL:O | 2.07 | 0.55 |
| 13:YB:57[E]:VAL:HG11 | 13:YB:75[E]:GLY:HA3 | 1.88 | 0.55 |
| 13:YC:214[D]:MET:HG2 | 13:YC:232[D]:ASN:O | 2.06 | 0.55 |
| 13:YC:425[A]:SER:HB2 | 13:YC:426[A]:PRO:HD2 | 1.89 | 0.55 |
| 13:YA:519[F]:THR:HA | 13:YC:527[F]:THR:O | 2.07 | 0.55 |
| 13:YC:89[C]:LYS:O | 13:YC:91[C]:LYS:HG3 | 2.06 | 0.55 |
| 14:YE:189[E]:TRP:NE1 | 14:YE:320[E]:PRO:HG2 | 2.21 | 0.55 |
| 14:YF:301[C]:MET:HA | 14:YF:304[C]:TYR:HD2 | 1.71 | 0.55 |
| 4:AA:42:PHE:O | 4:AA:62:HIS:ND1 | 2.27 | 0.55 |
| 5:AD:271:THR:HB | 5:AD:273:LYS:HG2 | 1.89 | 0.55 |
| 5:AD:36:GLU:HA | 5:AD:50:LYS:NZ | 2.22 | 0.55 |
| 5:AE:259:THR:OG1 | 5:AE:385:TRP:HB2 | 2.07 | 0.55 |
| 6:AH:23:LYS:HB3 | 6:AH:26:ASP:HB2 | 1.88 | 0.55 |
| 5:AC:356:TYR:CE1 | 6:AH:4:LEU:HD13 | 2.42 | 0.55 |
| 7:AI:497:ASN:H | 7:AI:500:TYR:HB2 | 1.71 | 0.55 |
| 7:AI:14:ARG:NH2 | 7:AJ:19:ASP:OD2 | 2.38 | 0.55 |
| 1:B:543:THR:HG21 | 1:B:551:GLY:CA | 2.37 | 0.55 |
| 7:AJ:36:ILE:HG13 | 7:BA:18:PHE:HE1 | 1.72 | 0.55 |
| 7:BA:330:ARG:NH2 | 7:BA:336:GLU:OE2 | 2.39 | 0.55 |
| 7:BA:392:LEU:HD22 | 7:BA:523:ILE:HG21 | 1.89 | 0.55 |
| 2:C:125:GLU:HG2 | 2:C:134:TYR:CG | 2.41 | 0.55 |
| 2:C:794:ASN:HB2 | 2:C:814:HIS:CE1 | 2.42 | 0.55 |
| 3:CA:263:LEU:HB2 | 3:CA:266:ASN:HB2 | 1.89 | 0.55 |
| 5:CF:146:VAL:HG21 | 5:CG:153:LYS:HD3 | 1.89 | 0.55 |
| 3:D:74:HIS:CE1 | 2:GF:449:LYS:HD2 | 2.42 | 0.55 |
| 7:DB:231:GLY:HA2 | 7:DC:222:GLU:HG3 | 1.89 | 0.55 |
| 11:DI:142:LYS:HB3 | 11:DI:143:TYR:HD2 | 1.71 | 0.55 |
| 12:DJ:149:ARG:HB3 | 10:GA:212:THR:HG21 | 1.89 | 0.55 |
| 12:DJ:165:ASP:OD1 | 12:DJ:166:SER:N | 2.40 | 0.55 |
| 1:EA:339:CYS:HB3 | 1:EA:348:PHE:CE2 | 2.42 | 0.55 |
| 1:EB:213:SER:OG | 1:EB:337:GLN:OE1 | 2.23 | 0.55 |
| 1:EB:386:THR:O | 1:EB:389:ARG:N | 2.39 | 0.55 |
| 1:EB:396:LEU:O | 1:EB:399:TYR:N | 2.40 | 0.55 |
| 2:EC:189:ARG:HG2 | 2:EC:204:ARG:NH1 | 2.22 | 0.55 |
| 2:EC:934:ALA:HB3 | 2:EC:997:SER:HB3 | 1.89 | 0.55 |
| 3:ED:24:PHE:O | 3:ED:27:SER:OG | 2.19 | 0.55 |
| 4:EG:67:TYR:HD1 | 4:EG:84:ARG:HB3 | 1.70 | 0.55 |
| 5:EI:103:ASN:OD1 | 5:EI:104:VAL:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:252:SER:OG | 5:EI:393:LEU:HB3 | 2.06 | 0.55 |
| 5:EJ:36:GLU:HA | 5:EJ:50:LYS:NZ | 2.22 | 0.55 |
| 5:EJ:290:SER:CB | 5:EJ:370:HIS:HA | 2.35 | 0.55 |
| 4:F:202:LEU:HA | 4:F:278:VAL:HA | 1.87 | 0.55 |
| 5:FA:3:GLN:HG3 | 5:FA:25:LYS:HG3 | 1.88 | 0.55 |
| 5:EJ:542:LEU:HD11 | 5:FA:569:TYR:CE2 | 2.41 | 0.55 |
| 7:FF:476:ASP:CG | 7:FF:479:ASN:HD21 | 2.09 | 0.55 |
| 7:FG:194:ALA:HB2 | 7:FG:208:TYR:HB3 | 1.88 | 0.55 |
| 7:FG:354:LEU:HG | 7:FG:361:PHE:CZ | 2.42 | 0.55 |
| 9:FJ:104:LEU:O | 9:FJ:126:LEU:N | 2.31 | 0.55 |
| 1:GD:147:SER:HA | 1:GD:167:LEU:HD23 | 1.88 | 0.55 |
| 1:GE:647:ARG:HD3 | 1:GE:650:TYR:HE2 | 1.71 | 0.55 |
| 2:GF:926:PRO:HD2 | 2:GF:985:GLU:O | 2.07 | 0.55 |
| 4:GJ:36:ASN:OD1 | 4:HA:7:LYS:NZ | 2.27 | 0.55 |
| 5:HB:200:LEU:HG | 5:HB:201:TYR:N | 2.22 | 0.55 |
| 5:HD:316:ILE:HG21 | 6:HF:7:LYS:HG3 | 1.89 | 0.55 |
| 7:HH:297:TYR:HB2 | 7:HJ:291:ARG:HA | 1.88 | 0.55 |
| 7:HH:359:TRP:NE1 | 7:HI:340:THR:O | 2.29 | 0.55 |
| 5:I:330:HIS:ND1 | 5:I:355:ASP:HB2 | 2.21 | 0.55 |
| 11:IE:142:LYS:HB3 | 11:IE:143:TYR:HD2 | 1.71 | 0.55 |
| 12:IF:165:ASP:OD1 | 12:IF:166:SER:N | 2.40 | 0.55 |
| 5:J:303:PRO:HB3 | 5:J:385:TRP:CZ2 | 2.42 | 0.55 |
| 5:K:206:PHE:CZ | 5:K:221:GLU:HG2 | 2.42 | 0.55 |
| 5:K:322:GLY:HA2 | 5:K:360:THR:H | 1.72 | 0.55 |
| 7:O:213:TYR:HB2 | 7:P:203:THR:O | 2.07 | 0.55 |
| 10:U:285:LEU:HA | 14:YD:215[A]:GLU:CG | 2.37 | 0.55 |
| 11:V:36:PHE:HZ | 11:V:76:CYS:HG | 1.53 | 0.55 |
| 1:X:345:TYR:OH | 1:X:400:ASN:OD1 | 2.25 | 0.55 |
| 1:X:88:SER:O | 1:X:91:GLN:N | 2.39 | 0.55 |
| 13:YA:58[B]:ILE:HG12 | 13:YA:97[B]:LEU:HD22 | 1.87 | 0.55 |
| 13:YA:61[E]:ILE:CG2 | 13:YB:59[E]:GLN:HA | 2.36 | 0.55 |
| 13:YA:89[A]:LYS:O | 13:YA:91[A]:LYS:HG3 | 2.06 | 0.55 |
| 13:YB:214[E]:MET:HG2 | 13:YB:232[E]:ASN:O | 2.06 | 0.55 |
| 13:YB:265[C]:VAL:HG22 | 13:YB:300[C]:LEU:HD23 | 1.88 | 0.55 |
| 13:YB:425[A]:SER:HB2 | 13:YB:426[A]:PRO:HD2 | 1.89 | 0.55 |
| 13:YA:442[E]:THR:HG21 | 13:YB:438[E]:LEU:HD22 | 1.88 | 0.55 |
| 13:YB:47[D]:ILE:HG23 | 14:YE:123[D]:PRO:CG | 2.30 | 0.55 |
| 13:YB:498[C]:VAL:HA | 13:YC:490[C]:VAL:O | 2.07 | 0.55 |
| 13:YB:565[A]:TYR:CZ | 13:YC:557[A]:MET:HG2 | 2.42 | 0.55 |
| 13:YB:89[E]:LYS:O | 13:YB:91[E]:LYS:HG3 | 2.06 | 0.55 |
| 13:YC:214[E]:MET:HG2 | 13:YC:232[E]:ASN:O | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:214[C]:MET:HG2 | 13:YC:232[C]:ASN:O | 2.06 | 0.55 |
| 13:YC:293[E]:ASN:O | 13:YC:297[E]:THR:N | 2.40 | 0.55 |
| 13:YA:534[A]:LEU:HD22 | 13:YC:538[A]:VAL:HG21 | 1.89 | 0.55 |
| 13:YA:534[E]:LEU:HD22 | 13:YC:538[E]:VAL:HG21 | 1.89 | 0.55 |
| 14:YD:178[E]:LEU:HD11 | 14:YD:183[E]:ASP:HA | 1.89 | 0.55 |
| 14:YE:156[B]:TYR:O | 14:YE:177[B]:ALA:HA | 2.07 | 0.55 |
| 14:YE:189[B]:TRP:NE1 | 14:YE:320[B]:PRO:HG2 | 2.21 | 0.55 |
| 14:YE:245[C]:ARG:HD3 | 14:YE:305[C]:ASP:OD2 | 2.06 | 0.55 |
| 14:YE:245[D]:ARG:HD3 | 14:YE:305[D]:ASP:OD2 | 2.06 | 0.55 |
| 14:YE:301[E]:MET:HA | 14:YE:304[E]:TYR:HD2 | 1.71 | 0.55 |
| 14:YF:245[A]:ARG:HD3 | 14:YF:305[A]:ASP:OD2 | 2.06 | 0.55 |
| 14:YF:30[C]:GLU:OE2 | 14:YF:31[C]:LEU:N | 2.40 | 0.55 |
| 14:YE:238[E]:THR:OG1 | 14:YF:92[E]:HIS:NE2 | 2.40 | 0.55 |
| 2:Z:406:LEU:HD11 | 2:Z:413:TRP:HA | 1.89 | 0.55 |
| 4:AB:201:LYS:HB3 | 4:AB:280:ALA:HB3 | 1.90 | 0.55 |
| 5:AD:256:SER:HB2 | 5:AD:387:ASN:OD1 | 2.07 | 0.55 |
| 6:AF:10:VAL:HG11 | 6:AH:10:VAL:HG21 | 1.89 | 0.55 |
| 1:B:441:ILE:HD11 | 1:B:644:ASN:ND2 | 2.21 | 0.55 |
| 7:AJ:192:GLN:NE2 | 7:BA:185:GLU:O | 2.33 | 0.55 |
| 8:BC:43:ALA:HB2 | 8:DF:139:GLU:H | 1.72 | 0.55 |
| 10:BE:210:ASP:HA | 10:BE:343:THR:HG22 | 1.89 | 0.55 |
| 12:BG:247:VAL:HG12 | 12:BG:248:MET:H | 1.71 | 0.55 |
| 1:BH:8:TYR:CZ | 1:BH:20:ILE:HG22 | 2.42 | 0.55 |
| 1:BH:5:PRO:HG2 | 2:BJ:674:TYR:HA | 1.89 | 0.55 |
| 1:BI:279:ASP:OD1 | 1:BI:280:ALA:N | 2.39 | 0.55 |
| 1:BI:543:THR:HG21 | 1:BI:551:GLY:CA | 2.37 | 0.55 |
| 2:BJ:825:GLU:N | 2:BJ:837:GLU:OE1 | 2.40 | 0.55 |
| 2:C:403:ILE:HD13 | 2:C:501:PHE:HE2 | 1.72 | 0.55 |
| 2:C:437:ASP:HA | 2:C:516:TRP:CE3 | 2.42 | 0.55 |
| 2:C:517:SER:O | 2:C:521:ASN:HA | 2.07 | 0.55 |
| 2:C:825:GLU:N | 2:C:837:GLU:OE1 | 2.40 | 0.55 |
| 5:CG:256:SER:HB2 | 5:CG:387:ASN:OD1 | 2.07 | 0.55 |
| 5:CH:206:PHE:CZ | 5:CH:221:GLU:HG2 | 2.42 | 0.55 |
| 7:DB:77:THR:HG23 | 7:DB:79:ALA:N | 2.22 | 0.55 |
| 7:DC:263:VAL:O | 7:DD:255:SER:OG | 2.14 | 0.55 |
| 7:DC:476:ASP:CG | 7:DC:479:ASN:HD21 | 2.09 | 0.55 |
| 8:BB:9:ALA:HB2 | 8:DE:34:PHE:HD2 | 1.72 | 0.55 |
| 2:BJ:654:PRO:HG3 | 9:DG:47:ARG:HD2 | 1.88 | 0.55 |
| 12:BG:137:TYR:CD2 | 12:DJ:221:ILE:HG12 | 2.42 | 0.55 |
| 2:C:790:THR:HA | 3:E:82:LEU:HD13 | 1.88 | 0.55 |
| 2:EC:926:PRO:HD2 | 2:EC:985:GLU:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:EF:1:MET:HG2 | 4:EF:70:HIS:CE1 | 2.41 | 0.55 |
| 5:EI:162:VAL:O | 5:EJ:253:GLN:HA | 2.06 | 0.55 |
| 5:EI:358:VAL:HG22 | 5:EI:371:PHE:HB2 | 1.88 | 0.55 |
| 5:FA:275:SER:OG | 5:FA:282:VAL:N | 2.40 | 0.55 |
| 8:FI:9:ALA:HB2 | 8:IB:34:PHE:HD2 | 1.71 | 0.55 |
| 11:GB:133:TRP:CZ2 | 11:GB:150:LEU:HD11 | 2.42 | 0.55 |
| 12:GC:222:SER:O | 12:GC:242:THR:N | 2.39 | 0.55 |
| 1:GD:341:THR:HG22 | 1:GD:343:THR:H | 1.71 | 0.55 |
| 1:GD:9:GLN:OE1 | 1:GD:9:GLN:N | 2.39 | 0.55 |
| 2:GF:808:GLN:NE2 | 2:GF:839:ILE:HG13 | 2.21 | 0.55 |
| 3:GH:46:PRO:HA | 3:GH:270:ARG:NH2 | 2.21 | 0.55 |
| 4:H:154:ASP:HB2 | 4:H:157:THR:HB | 1.88 | 0.55 |
| 5:HC:569:TYR:HE1 | 5:HD:544:VAL:HG22 | 1.71 | 0.55 |
| 5:HC:90:ASN:HA | 5:HD:98:VAL:HG22 | 1.89 | 0.55 |
| 7:HH:439:ILE:HG23 | 7:HJ:515:TRP:CH2 | 2.42 | 0.55 |
| 7:HI:12:GLU:HG3 | 7:HI:15:TYR:H | 1.71 | 0.55 |
| 7:HI:384:GLY:O | 7:HI:391:GLY:N | 2.36 | 0.55 |
| 7:HI:418:ASP:OD1 | 7:HI:422:LYS:N | 2.38 | 0.55 |
| 7:HJ:233:GLN:HE21 | 7:HJ:237:ASN:ND2 | 2.04 | 0.55 |
| 7:HJ:255:SER:HB3 | 7:HJ:263:VAL:HG13 | 1.89 | 0.55 |
| 5:I:293:PHE:HD1 | 5:I:298:LEU:HD11 | 1.71 | 0.55 |
| 5:J:202:TYR:HE1 | 5:J:206:PHE:HD1 | 1.54 | 0.55 |
| 5:K:289:LYS:HE2 | 5:K:370:HIS:CE1 | 2.42 | 0.55 |
| 7:P:476:ASP:CG | 7:P:479:ASN:HD21 | 2.09 | 0.55 |
| 7:P:99:ARG:NH1 | 7:P:101:SER:HB3 | 2.22 | 0.55 |
| 1:X:145:PHE:CZ | 1:X:286:PHE:HE1 | 2.24 | 0.55 |
| 1:X:339:CYS:HB3 | 1:X:348:PHE:CE2 | 2.42 | 0.55 |
| 1:Y:396:LEU:O | 1:Y:399:TYR:N | 2.40 | 0.55 |
| 13:YA:214[B]:MET:HG2 | 13:YA:232[B]:ASN:O | 2.06 | 0.55 |
| 13:YA:214[C]:MET:HG2 | 13:YA:232[C]:ASN:O | 2.06 | 0.55 |
| 13:YA:265[F]:VAL:HG22 | 13:YA:300[F]:LEU:HD23 | 1.88 | 0.55 |
| 13:YA:442[B]:THR:HG21 | 13:YB:438[B]:LEU:HD22 | 1.88 | 0.55 |
| 13:YB:25[E]:GLY:HA3 | 13:YB:73[E]:VAL:HG12 | 1.90 | 0.55 |
| 13:YB:82[C]:VAL:HG22 | 13:YB:98[C]:GLY:O | 2.07 | 0.55 |
| 13:YB:58[B]:ILE:HG12 | 13:YB:97[B]:LEU:HD22 | 1.88 | 0.55 |
| 13:YC:265[B]:VAL:HG22 | 13:YC:300[B]:LEU:HD23 | 1.88 | 0.55 |
| 13:YC:293[B]:ASN:O | 13:YC:297[B]:THR:N | 2.40 | 0.55 |
| 13:YC:293[C]:ASN:O | 13:YC:297[C]:THR:N | 2.39 | 0.55 |
| 13:YB:284[E]:MET:HE3 | 13:YC:363[E]:PRO:CB | 2.35 | 0.55 |
| 13:YA:519[A]:THR:HA | 13:YC:527[A]:THR:O | 2.07 | 0.55 |
| 13:YB:572[A]:ILE:HA | 13:YC:565[A]:TYR:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:572[D]:ILE:HA | 13:YC:565[D]:TYR:O | 2.06 | 0.55 |
| 13:YC:25[E]:GLY:HA3 | 13:YC:73[E]:VAL:HG12 | 1.90 | 0.55 |
| 13:YB:7[A]:ASN:ND2 | 13:YC:9[A]:ASN:HA | 2.14 | 0.55 |
| 14:YD:189[A]:TRP:NE1 | 14:YD:320[A]:PRO:HG2 | 2.21 | 0.55 |
| 14:YD:301[A]:MET:HA | 14:YD:304[A]:TYR:HD2 | 1.71 | 0.55 |
| 14:YF:292[F]:TYR:CD1 | 14:YF:371[F]:LYS:HB3 | 2.42 | 0.55 |
| 2:Z:450:PHE:CZ | 2:Z:473:TYR:CE1 | 2.94 | 0.55 |
| 2:Z:653:MET:HB3 | 2:Z:658:LEU:HD11 | 1.89 | 0.55 |
| 1:A:448:TYR:CZ | 1:A:642:PHE:HB2 | 2.41 | 0.54 |
| 5:AC:330:HIS:ND1 | 5:AC:355:ASP:HB2 | 2.21 | 0.54 |
| 5:AD:44:TYR:CD2 | 5:AD:48:ALA:HB2 | 2.37 | 0.54 |
| 5:AE:212:PHE:CZ | 5:AE:230:ILE:HB | 2.41 | 0.54 |
| 5:AE:18:TYR:HB2 | 5:AE:21:LYS:H | 1.71 | 0.54 |
| 5:AE:419:ASP:HB3 | 5:AE:436:VAL:HB | 1.89 | 0.54 |
| 1:BI:510:MET:HB3 | 1:BI:542:SER:HB3 | 1.89 | 0.54 |
| 2:BJ:517:SER:O | 2:BJ:521:ASN:HA | 2.06 | 0.54 |
| 2:BJ:794:ASN:HB2 | 2:BJ:814:HIS:CE1 | 2.42 | 0.54 |
| 2:C:172:GLU:HA | 3:D:166:SER:H | 74.25 | 0.54 |
| 2:C:339:ASP:HB3 | 2:C:340:PRO:CD | 2.36 | 0.54 |
| 4:CD:201:LYS:HB3 | 4:CD:280:ALA:HB3 | 1.90 | 0.54 |
| 4:CD:36:ASN:OD1 | 4:CE:7:LYS:NZ | 2.29 | 0.54 |
| 5:CF:339:GLU:HB3 | 6:CJ:172:SER:O | 2.07 | 0.54 |
| 5:CG:118:LYS:HA | 5:CG:142:ARG:NH2 | 2.22 | 0.54 |
| 5:CH:353:HIS:NE2 | 7:HJ:476:ASP:HB2 | 2.22 | 0.54 |
| 3:D:226:GLU:OE1 | 3:D:226:GLU:N | 2.34 | 0.54 |
| 7:DD:383:TYR:CD1 | 7:DD:393:PRO:HG3 | 2.42 | 0.54 |
| 7:DB:447:HIS:CD2 | 7:DD:447:HIS:HD2 | 2.25 | 0.54 |
| 12:DJ:222:SER:O | 12:DJ:242:THR:N | 2.39 | 0.54 |
| 3:E:150:LYS:HA | 3:E:160:TRP:CE3 | 2.42 | 0.54 |
| 2:C:900:ILE:HG13 | 3:E:311:TYR:CE1 | 2.43 | 0.54 |
| 1:EA:345:TYR:OH | 1:EA:400:ASN:OD1 | 2.25 | 0.54 |
| 1:EB:647:ARG:HD3 | 1:EB:650:TYR:HE2 | 1.71 | 0.54 |
| 2:EC:143:MET:HG2 | 2:EC:544:VAL:HG22 | 1.87 | 0.54 |
| 2:EC:182:GLN:O | 2:EC:210:LYS:NZ | 2.33 | 0.54 |
| 3:ED:261:ALA:O | 3:ED:266:ASN:ND2 | 2.30 | 0.54 |
| 5:EI:535:THR:O | 5:FA:576:THR:N | 2.32 | 0.54 |
| 5:EJ:312:ARG:O | 5:EJ:382:ASN:N | 2.30 | 0.54 |
| 5:FA:168:LEU:HA | 5:FA:241:THR:HG22 | 1.87 | 0.54 |
| 5:FA:259:THR:OG1 | 5:FA:385:TRP:HB2 | 2.07 | 0.54 |
| 5:FA:264:ARG:HG3 | 5:FA:379:ASP:O | 2.07 | 0.54 |
| 7:FF:349:TRP:N | 7:FF:520:ASN:O | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:449:GLY:N | 7:FG:482:TYR:O | 2.31 | 0.54 |
| 8:FI:130:LYS:NZ | 8:FI:163:GLU:OE2 | 2.37 | 0.54 |
| 11:GB:57:GLU:OE1 | 11:GB:57:GLU:N | 2.25 | 0.54 |
| 1:GE:396:LEU:O | 1:GE:399:TYR:N | 2.40 | 0.54 |
| 1:GE:543:THR:HG21 | 1:GE:551:GLY:CA | 2.37 | 0.54 |
| 1:GE:544:ASP:CB | 1:GE:576:ASP:HB2 | 2.36 | 0.54 |
| 1:GE:441:ILE:HD11 | 1:GE:644:ASN:ND2 | 2.21 | 0.54 |
| 1:GE:76:TYR:HB3 | 1:GE:82:THR:HG21 | 1.87 | 0.54 |
| 2:GF:189:ARG:HG2 | 2:GF:204:ARG:NH1 | 2.22 | 0.54 |
| 2:GF:422:GLU:HB3 | 2:GF:423:GLU:OE1 | 2.06 | 0.54 |
| 2:GF:738:LYS:HD2 | 2:GF:882:PHE:O | 2.06 | 0.54 |
| 2:GF:934:ALA:HB3 | 2:GF:997:SER:HB3 | 1.89 | 0.54 |
| 4:GI:39:TYR:CD1 | 4:GJ:7:LYS:HB2 | 2.42 | 0.54 |
| 5:HB:146:VAL:HG21 | 5:HC:153:LYS:HD3 | 1.89 | 0.54 |
| 5:HC:358:VAL:HG22 | 5:HC:371:PHE:HB2 | 1.89 | 0.54 |
| 7:HJ:330:ARG:NH2 | 7:HJ:336:GLU:OE2 | 2.40 | 0.54 |
| 7:HI:515:TRP:CZ2 | 7:HJ:439:ILE:HG23 | 2.42 | 0.54 |
| 5:K:264:ARG:HG3 | 5:K:379:ASP:O | 2.07 | 0.54 |
| 7:O:130:GLU:HA | 7:P:139:ASN:HD21 | 1.72 | 0.54 |
| 7:O:77:THR:HG23 | 7:O:79:ALA:N | 2.22 | 0.54 |
| 7:P:36:ILE:HG13 | 7:Q:18:PHE:HE1 | 1.72 | 0.54 |
| 10:U:341:THR:HG22 | 10:U:343:THR:H | 8.30 | 0.54 |
| 12:W:165:ASP:OD1 | 12:W:166:SER:N | 2.40 | 0.54 |
| 13:YA:527[E]:THR:O | 13:YB:519[E]:THR:HA | 2.06 | 0.54 |
| 13:YB:265[E]:VAL:HG22 | 13:YB:300[E]:LEU:HD23 | 1.88 | 0.54 |
| 13:YA:503[E]:THR:O | 13:YB:495[E]:THR:HA | 2.06 | 0.54 |
| 13:YC:265[C]:VAL:HG22 | 13:YC:300[C]:LEU:HD23 | 1.88 | 0.54 |
| 13:YB:284[D]:MET:HE3 | 13:YC:363[D]:PRO:CB | 2.35 | 0.54 |
| 13:YB:474[E]:ILE:HD11 | 13:YC:470[E]:ARG:HD2 | 1.89 | 0.54 |
| 13:YA:534[C]:LEU:HD22 | 13:YC:538[C]:VAL:HG21 | 1.89 | 0.54 |
| 14:YD:156[E]:TYR:O | 14:YD:177[E]:ALA:HA | 2.06 | 0.54 |
| 14:YD:30[B]:GLU:OE2 | 14:YD:31[B]:LEU:N | 2.40 | 0.54 |
| 14:YD:30[A]:GLU:OE2 | 14:YD:31[A]:LEU:N | 2.40 | 0.54 |
| 14:YE:178[C]:LEU:HD11 | 14:YE:183[C]:ASP:HA | 1.89 | 0.54 |
| 14:YE:189[A]:TRP:NE1 | 14:YE:320[A]:PRO:HG2 | 2.21 | 0.54 |
| 14:YE:30[E]:GLU:OE2 | 14:YE:31[E]:LEU:N | 2.40 | 0.54 |
| 14:YE:30[B]:GLU:OE2 | 14:YE:31[B]:LEU:N | 2.40 | 0.54 |
| 14:YE:30[C]:GLU:OE2 | 14:YE:31[C]:LEU:N | 2.40 | 0.54 |
| 14:YF:178[A]:LEU:HD11 | 14:YF:183[A]:ASP:HA | 1.89 | 0.54 |
| 14:YF:189[E]:TRP:NE1 | 14:YF:320[E]:PRO:HG2 | 2.21 | 0.54 |
| 14:YF:189[F]:TRP:NE1 | 14:YF:320[F]:PRO:HG2 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:30[A]:GLU:OE2 | 14:YF:31[A]:LEU:N | 2.40 | 0.54 |
| 14:YD:101[A]:GLY:HA2 | 14:YF:332[A]:GLN:OE1 | 2.07 | 0.54 |
| 2:Z:356:THR:OG1 | 2:Z:357:ILE:O | 2.21 | 0.54 |
| 2:Z:935:LYS:HZ3 | 2:Z:936:LEU:HD13 | 1.71 | 0.54 |
| 1:A:117:ALA:HB1 | 2:Z:947:VAL:O | 177.39 | 0.54 |
| 1:A:145:PHE:CZ | 1:A:286:PHE:HE1 | 2.24 | 0.54 |
| 1:A:8:TYR:CZ | 1:A:20:ILE:HG22 | 2.42 | 0.54 |
| 4:AA:201:LYS:HB3 | 4:AA:280:ALA:HB3 | 1.90 | 0.54 |
| 5:AD:117:ILE:HG22 | 5:AD:143:TRP:CE3 | 2.42 | 0.54 |
| 5:AD:202:TYR:HE1 | 5:AD:206:PHE:HD1 | 1.54 | 0.54 |
| 5:AE:264:ARG:HG3 | 5:AE:379:ASP:O | 2.07 | 0.54 |
| 5:AE:39:ASP:HB2 | 5:AE:44:TYR:HE2 | 1.72 | 0.54 |
| 6:AF:100:PRO:O | 6:AF:103:SER:OG | 2.18 | 0.54 |
| 7:AJ:99:ARG:NH1 | 7:AJ:101:SER:HB3 | 2.22 | 0.54 |
| 7:AJ:289:GLN:OE1 | 7:AJ:294:GLN:NE2 | 2.40 | 0.54 |
| 1:B:196:GLN:HG3 | 1:B:273:ILE:HD12 | 1.88 | 0.54 |
| 1:BH:403:PRO:HG3 | 1:BI:404:ILE:HD12 | 1.88 | 0.54 |
| 2:BJ:794:ASN:HB2 | 2:BJ:814:HIS:NE2 | 2.22 | 0.54 |
| 2:BJ:934:ALA:HB3 | 2:BJ:997:SER:HB3 | 1.89 | 0.54 |
| 2:C:153:PHE:O | 2:C:154:SER:OG | 2.25 | 0.54 |
| 2:C:794:ASN:HB2 | 2:C:814:HIS:NE2 | 2.22 | 0.54 |
| 2:C:919:TYR:HA | 2:C:990:MET:HE3 | 1.88 | 0.54 |
| 5:CF:63:GLU:HB2 | 5:CF:68:TYR:OH | 2.07 | 0.54 |
| 5:CH:39:ASP:HB2 | 5:CH:44:TYR:HE2 | 1.72 | 0.54 |
| 5:CH:60:LEU:HG | 5:CH:79:ILE:HG22 | 1.88 | 0.54 |
| 6:CI:23:LYS:HB3 | 6:CI:26:ASP:HB2 | 1.88 | 0.54 |
| 6:CJ:69:THR:HA | 6:DA:73:ASN:HB3 | 1.89 | 0.54 |
| 3:D:263:LEU:HB2 | 3:D:266:ASN:HB2 | 1.89 | 0.54 |
| 7:DB:12:GLU:HG3 | 7:DB:14:ARG:H | 1.71 | 0.54 |
| 7:DC:289:GLN:OE1 | 7:DC:294:GLN:NE2 | 2.40 | 0.54 |
| 7:DC:515:TRP:CZ2 | 7:DD:439:ILE:HG23 | 2.42 | 0.54 |
| 4:EG:53:GLY:O | 4:EH:7:LYS:HB3 | 2.07 | 0.54 |
| 5:EI:200:LEU:HG | 5:EI:201:TYR:N | 2.22 | 0.54 |
| 4:F:39:TYR:CD1 | 4:G:7:LYS:HB2 | 2.41 | 0.54 |
| 5:FA:60:LEU:HG | 5:FA:79:ILE:HG22 | 1.88 | 0.54 |
| 5:EJ:356:TYR:HE1 | 6:FB:4:LEU:HD13 | 1.72 | 0.54 |
| 7:FE:77:THR:HG23 | 7:FE:79:ALA:N | 2.22 | 0.54 |
| 7:FF:63:GLU:O | 7:FF:67:ILE:HG12 | 2.08 | 0.54 |
| 4:F:53:GLY:HA3 | 4:G:7:LYS:HE2 | 1.90 | 0.54 |
| 1:GE:229:THR:OG1 | 1:GE:233:ASN:O | 2.23 | 0.54 |
| 2:GF:153:PHE:O | 2:GF:154:SER:OG | 2.25 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:437:ASP:HA | 2:GF:516:TRP:CE3 | 2.42 | 0.54 |
| 2:GF:575:PHE:O | 2:GF:607:THR:OG1 | 2.13 | 0.54 |
| 2:GF:909:THR:OG1 | 2:GF:910:GLU:OE1 | 2.11 | 0.54 |
| 4:G:172:GLU:HA | 4:H:166:SER:H | 1.73 | 0.54 |
| 5:HB:358:VAL:HG22 | 5:HB:371:PHE:HB2 | 1.88 | 0.54 |
| 5:HC:303:PRO:HB3 | 5:HC:385:TRP:CZ2 | 2.42 | 0.54 |
| 5:HD:185:SER:HB2 | 5:HD:228:PHE:HE1 | 1.72 | 0.54 |
| 5:HD:322:GLY:HA2 | 5:HD:360:THR:H | 1.72 | 0.54 |
| 5:HD:259:THR:OG1 | 5:HD:385:TRP:HB2 | 2.07 | 0.54 |
| 5:HD:60:LEU:HG | 5:HD:79:ILE:HG22 | 1.88 | 0.54 |
| 7:HH:289:GLN:OE1 | 7:HH:294:GLN:NE2 | 2.40 | 0.54 |
| 7:HH:29:ILE:HG22 | 7:HH:30:THR:N | 2.14 | 0.54 |
| 5:I:255:ARG:CZ | 5:K:390:LEU:HD12 | 2.36 | 0.54 |
| 5:I:265:LEU:HG | 5:I:379:ASP:HB2 | 1.90 | 0.54 |
| 8:FI:43:ALA:HB2 | 8:IB:139:GLU:H | 1.72 | 0.54 |
| 5:J:65:GLY:O | 5:K:45:SER:OG | 2.12 | 0.54 |
| 5:K:3:GLN:HG3 | 5:K:25:LYS:HG3 | 1.88 | 0.54 |
| 5:K:563:GLY:O | 5:K:565:ILE:N | 2.34 | 0.54 |
| 7:O:447:HIS:CD2 | 7:P:447:HIS:CD2 | 2.96 | 0.54 |
| 7:O:100:TYR:OH | 7:P:113:GLU:HG3 | 2.08 | 0.54 |
| 7:P:12:GLU:HG3 | 7:P:15:TYR:H | 1.71 | 0.54 |
| 7:Q:354:LEU:HG | 7:Q:361:PHE:CZ | 2.42 | 0.54 |
| 7:Q:383:TYR:CD1 | 7:Q:393:PRO:HG3 | 2.41 | 0.54 |
| 8:R:10:PHE:C | 8:R:12:SER:H | 2.08 | 0.54 |
| 1:X:307:ASP:HB3 | 1:X:309:ASP:N | 2.22 | 0.54 |
| 13:YA:293[E]:ASN:O | 13:YA:297[E]:THR:N | 2.40 | 0.54 |
| 13:YA:265[A]:VAL:HG22 | 13:YA:300[A]:LEU:HD23 | 1.88 | 0.54 |
| 13:YB:265[D]:VAL:HG22 | 13:YB:300[D]:LEU:HD23 | 1.88 | 0.54 |
| 13:YB:437[C]:ASN:HB3 | 13:YB:439[C]:TYR:CE1 | 2.43 | 0.54 |
| 13:YA:527[D]:THR:O | 13:YB:519[D]:THR:HA | 2.05 | 0.54 |
| 13:YC:437[F]:ASN:HB3 | 13:YC:439[F]:TYR:CE1 | 2.42 | 0.54 |
| 13:YB:474[A]:ILE:HD11 | 13:YC:470[A]:ARG:HD2 | 1.89 | 0.54 |
| 13:YA:519[D]:THR:HA | 13:YC:527[D]:THR:O | 2.07 | 0.54 |
| 13:YA:534[D]:LEU:HD22 | 13:YC:538[D]:VAL:HG21 | 1.89 | 0.54 |
| 13:YC:90[A]:TRP:NE1 | 14:YF:175[A]:GLU:OE1 | 2.35 | 0.54 |
| 14:YD:30[D]:GLU:OE2 | 14:YD:31[D]:LEU:N | 2.40 | 0.54 |
| 14:YD:30[E]:GLU:OE2 | 14:YD:31[E]:LEU:N | 2.40 | 0.54 |
| 14:YE:30[F]:GLU:OE2 | 14:YE:31[F]:LEU:N | 2.40 | 0.54 |
| 14:YE:332[E]:GLN:OE1 | 14:YF:101[E]:GLY:HA2 | 2.08 | 0.54 |
| 14:YF:245[B]:ARG:HD3 | 14:YF:305[B]:ASP:OD2 | 2.06 | 0.54 |
| 14:YF:30[D]:GLU:OE2 | 14:YF:31[D]:LEU:N | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:30[F]:GLU:OE2 | 14:YF:31[F]:LEU:N | 2.40 | 0.54 |
| 2:Z:964:PRO:HG2 | 2:Z:966:PRO:HG3 | 1.89 | 0.54 |
| 2:Z:926:PRO:HD2 | 2:Z:985:GLU:O | 2.07 | 0.54 |
| 15:ZA:16[D]:ALA:HB3 | 15:ZA:48[D]:GLU:HB2 | 1.89 | 0.54 |
| 15:ZA:76[D]:GLN:HB3 | 15:ZA:96[D]:ILE:HD11 | 1.90 | 0.54 |
| 1:A:388:GLN:O | 1:A:392:ILE:HG22 | 2.06 | 0.54 |
| 5:AD:94:ARG:HD3 | 5:AD:134:GLU:HG2 | 1.89 | 0.54 |
| 5:AE:206:PHE:CZ | 5:AE:221:GLU:HG2 | 2.42 | 0.54 |
| 5:AE:285:LEU:CD1 | 5:AE:375:PHE:HB2 | 2.36 | 0.54 |
| 7:AI:213:TYR:HB2 | 7:AJ:203:THR:O | 2.07 | 0.54 |
| 7:AI:297:TYR:HB2 | 7:BA:291:ARG:HA | 1.89 | 0.54 |
| 7:AJ:93:THR:HG22 | 7:AJ:94:VAL:HG23 | 1.89 | 0.54 |
| 7:BA:29:ILE:O | 7:BA:30:THR:OG1 | 2.19 | 0.54 |
| 8:BB:69:TRP:HZ3 | 8:BB:157:LEU:HD12 | 1.72 | 0.54 |
| 11:BF:61:ASN:O | 11:BF:65:GLY:N | 2.38 | 0.54 |
| 2:BJ:184:CYS:O | 2:BJ:185:LYS:HG2 | 2.07 | 0.54 |
| 2:BJ:189:ARG:HG2 | 2:BJ:204:ARG:NH1 | 2.22 | 0.54 |
| 2:C:174:HIS:CG | 2:C:508:TYR:HH | 2.25 | 0.54 |
| 2:C:158:VAL:O | 2:C:593:GLU:HA | 2.08 | 0.54 |
| 4:CC:1:MET:HG2 | 4:CC:70:HIS:CE1 | 2.41 | 0.54 |
| 5:CF:358:VAL:HG22 | 5:CF:371:PHE:HB2 | 1.88 | 0.54 |
| 5:CH:172:GLN:HG2 | 5:CH:173:GLY:H | 1.73 | 0.54 |
| 5:CH:185:SER:HB2 | 5:CH:228:PHE:HE1 | 1.72 | 0.54 |
| 6:CJ:135:GLU:HA | 6:CJ:138:ALA:HB3 | 1.89 | 0.54 |
| 7:DC:384:GLY:O | 7:DC:391:GLY:N | 2.36 | 0.54 |
| 7:DB:56:GLY:CA | 7:DD:57:ILE:HG23 | 2.38 | 0.54 |
| 8:DE:69:TRP:HZ3 | 8:DE:157:LEU:HD12 | 1.72 | 0.54 |
| 10:DH:210:ASP:HA | 10:DH:343:THR:HG22 | 1.90 | 0.54 |
| 2:EC:153:PHE:O | 2:EC:154:SER:OG | 2.25 | 0.54 |
| 2:EC:158:VAL:O | 2:EC:593:GLU:HA | 2.08 | 0.54 |
| 2:EC:504:GLN:CD | 2:EC:505:PRO:HD2 | 2.27 | 0.54 |
| 2:EC:794:ASN:HB2 | 2:EC:814:HIS:NE2 | 2.22 | 0.54 |
| 3:EE:254:ASP:OD1 | 3:EE:255:SER:N | 2.41 | 0.54 |
| 4:EF:154:ASP:HB2 | 4:EF:157:THR:HB | 1.88 | 0.54 |
| 4:EG:201:LYS:HB3 | 4:EG:280:ALA:HB3 | 1.90 | 0.54 |
| 4:EH:111:ASN:HD21 | 4:EH:116:ILE:H | 1.56 | 0.54 |
| 5:EI:568:LYS:HA | 5:EJ:550:VAL:O | 2.07 | 0.54 |
| 5:EJ:118:LYS:HA | 5:EJ:142:ARG:NH2 | 2.22 | 0.54 |
| 5:EJ:490:TRP:NE1 | 5:EJ:515:THR:O | 2.40 | 0.54 |
| 5:FA:415:ASP:HB2 | 5:FA:440:GLN:HE22 | 1.71 | 0.54 |
| 7:FG:330:ARG:NH2 | 7:FG:336:GLU:OE2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:448:TYR:CZ | 1:GD:642:PHE:HB2 | 2.41 | 0.54 |
| 1:GE:279:ASP:OD1 | 1:GE:280:ALA:N | 2.39 | 0.54 |
| 1:GE:70:PHE:HE2 | 2:GF:686:LEU:CB | 2.17 | 0.54 |
| 2:GF:403:ILE:HD13 | 2:GF:501:PHE:HE2 | 1.72 | 0.54 |
| 2:GF:548:ILE:HB | 2:GF:555:ARG:HB3 | 1.89 | 0.54 |
| 3:GG:195:PRO:HG3 | 3:GG:222:ARG:HD3 | 1.89 | 0.54 |
| 4:GJ:1:MET:HG2 | 4:GJ:70:HIS:CE1 | 2.41 | 0.54 |
| 5:HC:13:ASP:OD1 | 5:HC:14:GLY:N | 2.41 | 0.54 |
| 5:HC:137:TYR:HA | 5:HC:143:TRP:HD1 | 1.73 | 0.54 |
| 5:HD:172:GLN:HG2 | 5:HD:173:GLY:H | 1.73 | 0.54 |
| 5:HD:212:PHE:CZ | 5:HD:230:ILE:HB | 2.41 | 0.54 |
| 7:HH:99:ARG:NH1 | 7:HH:105:GLU:OE2 | 2.32 | 0.54 |
| 6:FB:140:PHE:CZ | 7:HI:196:VAL:HG11 | 2.41 | 0.54 |
| 7:HH:112:ASN:HA | 7:HJ:117:THR:OG1 | 2.07 | 0.54 |
| 7:HJ:194:ALA:HB2 | 7:HJ:208:TYR:HB3 | 1.88 | 0.54 |
| 7:HJ:20:PRO:HG3 | 7:HJ:29:ILE:HG13 | 1.89 | 0.54 |
| 5:I:200:LEU:HG | 5:I:201:TYR:N | 2.22 | 0.54 |
| 5:J:102:TRP:CE3 | 5:J:131:SER:HB2 | 2.43 | 0.54 |
| 2:C:984:SER:OG | 5:J:12:ASP:OD2 | 2.13 | 0.54 |
| 5:K:289:LYS:O | 5:K:290:SER:OG | 2.25 | 0.54 |
| 5:K:316:ILE:HG21 | 6:M:7:LYS:HG3 | 1.88 | 0.54 |
| 5:K:419:ASP:HB3 | 5:K:436:VAL:HB | 1.89 | 0.54 |
| 5:K:60:LEU:HG | 5:K:79:ILE:HG22 | 1.88 | 0.54 |
| 6:L:29:VAL:O | 6:L:32:ARG:N | 2.36 | 0.54 |
| 5:I:340:VAL:HG21 | 6:M:174:TYR:H | 1.72 | 0.54 |
| 7:O:12:GLU:HG3 | 7:O:14:ARG:H | 1.71 | 0.54 |
| 7:O:386:ASN:HB2 | 7:O:387:PRO:HD2 | 1.90 | 0.54 |
| 11:V:133:TRP:CZ2 | 11:V:150:LEU:HD11 | 2.42 | 0.54 |
| 1:X:282:GLY:N | 1:X:312:GLY:O | 2.39 | 0.54 |
| 1:Y:543:THR:HG21 | 1:Y:551:GLY:CA | 2.37 | 0.54 |
| 13:YA:437[E]:ASN:HB3 | 13:YA:439[E]:TYR:CE1 | 2.43 | 0.54 |
| 13:YA:437[F]:ASN:HB3 | 13:YA:439[F]:TYR:CE1 | 2.42 | 0.54 |
| 13:YA:554[D]:MET:HE2 | 13:YB:550[D]:TRP:CD1 | 2.42 | 0.54 |
| 13:YA:61[F]:ILE:HG12 | 13:YB:60[F]:PRO:CD | 2.38 | 0.54 |
| 13:YA:18[E]:ARG:NH1 | 13:YA:77[E]:VAL:HG23 | 2.23 | 0.54 |
| 13:YC:193[F]:ASP:OD1 | 13:YC:197[F]:TYR:N | 2.31 | 0.54 |
| 13:YA:466[F]:ASN:HB2 | 13:YC:474[F]:ILE:HG12 | 1.89 | 0.54 |
| 13:YA:76[A]:PRO:HA | 13:YC:61[A]:ILE:HA | 1.90 | 0.54 |
| 13:YC:18[E]:ARG:NH1 | 13:YC:77[E]:VAL:HG23 | 2.23 | 0.54 |
| 14:YD:238[B]:THR:OG1 | 14:YE:92[B]:HIS:NE2 | 2.41 | 0.54 |
| 14:YD:92[A]:HIS:NE2 | 14:YF:238[A]:THR:OG1 | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:238[C]:THR:OG1 | 14:YE:92[C]:HIS:NE2 | 2.40 | 0.54 |
| 14:YF:156[A]:TYR:O | 14:YF:177[A]:ALA:HA | 2.07 | 0.54 |
| 14:YF:189[D]:TRP:NE1 | 14:YF:320[D]:PRO:HG2 | 2.21 | 0.54 |
| 2:Z:184:CYS:O | 2:Z:185:LYS:HG2 | 2.07 | 0.54 |
| 4:AB:154:ASP:HB2 | 4:AB:157:THR:HB | 1.88 | 0.54 |
| 4:AA:171:LYS:HB2 | 4:AB:165:GLU:HB3 | 1.89 | 0.54 |
| 5:AC:372:ASP:OD1 | 5:AC:372:ASP:N | 2.40 | 0.54 |
| 6:AF:135:GLU:HA | 6:AF:138:ALA:HB3 | 1.89 | 0.54 |
| 6:AG:54:SER:O | 6:AH:164:GLN:NE2 | 2.40 | 0.54 |
| 7:AI:77:THR:HG23 | 7:AI:79:ALA:N | 2.22 | 0.54 |
| 7:AI:118:PRO:HG3 | 7:AJ:106:ALA:HA | 1.90 | 0.54 |
| 7:BA:20:PRO:HG3 | 7:BA:29:ILE:HG13 | 1.89 | 0.54 |
| 8:BC:23:VAL:HA | 8:BC:113:VAL:HA | 1.90 | 0.54 |
| 2:C:969:TYR:O | 2:C:973:ASN:N | 2.29 | 0.54 |
| 5:CF:372:ASP:N | 5:CF:372:ASP:OD1 | 2.40 | 0.54 |
| 5:CG:304:ILE:HG13 | 5:CG:386:PHE:H | 1.72 | 0.54 |
| 5:CH:259:THR:OG1 | 5:CH:385:TRP:HB2 | 2.07 | 0.54 |
| 6:CJ:29:VAL:O | 6:CJ:32:ARG:N | 2.36 | 0.54 |
| 7:DB:322:THR:HG23 | 7:DC:327:GLN:HE21 | 1.73 | 0.54 |
| 1:EA:307:ASP:HB3 | 1:EA:309:ASP:N | 2.22 | 0.54 |
| 1:EB:543:THR:HG21 | 1:EB:551:GLY:CA | 2.37 | 0.54 |
| 2:EC:1005:ARG:HG3 | 5:EI:12:ASP:OD2 | 2.07 | 0.54 |
| 2:EC:148:ASN:HA | 2:EC:168:ILE:HD13 | 1.90 | 0.54 |
| 2:EC:39:ALA:HB1 | 2:EC:54:TYR:CE1 | 2.42 | 0.54 |
| 2:EC:450:PHE:CZ | 2:EC:473:TYR:CE1 | 2.94 | 0.54 |
| 2:EC:403:ILE:HD13 | 2:EC:501:PHE:HE2 | 1.72 | 0.54 |
| 2:EC:548:ILE:HB | 2:EC:555:ARG:HB3 | 1.89 | 0.54 |
| 4:EG:124:ILE:HD12 | 4:EG:137:LEU:HD23 | 1.90 | 0.54 |
| 4:EH:154:ASP:HB2 | 4:EH:157:THR:HB | 1.89 | 0.54 |
| 5:FA:39:ASP:HB2 | 5:FA:44:TYR:HE2 | 1.72 | 0.54 |
| 8:FH:82:ARG:HH12 | 8:FH:138:GLY:HA2 | 1.73 | 0.54 |
| 4:G:124:ILE:HD12 | 4:G:137:LEU:HD23 | 1.90 | 0.54 |
| 1:GD:231:ASP:OD1 | 1:GD:233:ASN:N | 2.36 | 0.54 |
| 1:GD:522:LYS:HB3 | 1:GD:533:ASP:HA | 1.90 | 0.54 |
| 2:GF:517:SER:O | 2:GF:521:ASN:HA | 2.07 | 0.54 |
| 4:GI:124:ILE:HD12 | 4:GI:137:LEU:HD23 | 1.90 | 0.54 |
| 4:GI:53:GLY:O | 4:GJ:7:LYS:HB3 | 2.07 | 0.54 |
| 4:H:201:LYS:HB3 | 4:H:280:ALA:HB3 | 1.90 | 0.54 |
| 5:HC:196:ARG:NE | 7:HJ:5:THR:HG23 | 2.23 | 0.54 |
| 5:HC:256:SER:HB2 | 5:HC:387:ASN:OD1 | 2.06 | 0.54 |
| 5:HC:330:HIS:ND1 | 5:HC:355:ASP:HB2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:39:ASP:HB2 | 5:HD:44:TYR:HE2 | 1.72 | 0.54 |
| 7:HH:447:HIS:CD2 | 7:HI:447:HIS:CD2 | 2.95 | 0.54 |
| 7:HJ:383:TYR:CD1 | 7:HJ:393:PRO:HG3 | 2.42 | 0.54 |
| 7:HH:441:GLN:N | 7:HJ:513:ARG:O | 2.34 | 0.54 |
| 8:FI:115:GLN:HG2 | 8:IB:79:HIS:HE2 | 1.73 | 0.54 |
| 7:O:29:ILE:O | 7:O:30:THR:OG1 | 2.23 | 0.54 |
| 7:P:515:TRP:CZ2 | 7:Q:439:ILE:HG23 | 2.42 | 0.54 |
| 7:O:56:GLY:CA | 7:Q:57:ILE:HG23 | 2.38 | 0.54 |
| 13:YA:214[F]:MET:HG2 | 13:YA:232[F]:ASN:O | 2.06 | 0.54 |
| 13:YA:293[A]:ASN:O | 13:YA:297[A]:THR:N | 2.40 | 0.54 |
| 13:YA:442[A]:THR:HG21 | 13:YB:438[A]:LEU:HD22 | 1.89 | 0.54 |
| 13:YA:26[F]:ARG:HA | 13:YA:55[F]:MET:O | 2.07 | 0.54 |
| 13:YA:82[C]:VAL:HG22 | 13:YA:98[C]:GLY:O | 2.08 | 0.54 |
| 13:YB:214[F]:MET:HG2 | 13:YB:232[F]:ASN:O | 2.06 | 0.54 |
| 13:YC:293[A]:ASN:O | 13:YC:297[A]:THR:N | 2.40 | 0.54 |
| 13:YC:31[C]:VAL:O | 13:YC:35[C]:HIS:HB2 | 2.08 | 0.54 |
| 13:YA:519[C]:THR:HA | 13:YC:527[C]:THR:O | 2.07 | 0.54 |
| 14:YD:189[B]:TRP:NE1 | 14:YD:320[B]:PRO:HG2 | 2.21 | 0.54 |
| 10:BE:285:LEU:HA | 14:YD:215[C]:GLU:CG | 2.37 | 0.54 |
| 14:YF:30[B]:GLU:OE2 | 14:YF:31[B]:LEU:N | 2.40 | 0.54 |
| 14:YF:43[F]:SER:OG | 14:YF:45[F]:TYR:N | 2.40 | 0.54 |
| 5:AD:67:SER:HB2 | 5:AD:94:ARG:HB2 | 1.90 | 0.54 |
| 6:AF:10:VAL:CG1 | 6:AH:10:VAL:HG21 | 2.38 | 0.54 |
| 7:AI:386:ASN:HB2 | 7:AI:387:PRO:HD2 | 1.90 | 0.54 |
| 7:AJ:295:ILE:HG13 | 7:BA:301:ARG:HB3 | 1.88 | 0.54 |
| 1:B:23:GLY:H | 11:V:26:THR:HG1 | 1.53 | 0.54 |
| 1:B:396:LEU:O | 1:B:399:TYR:N | 2.40 | 0.54 |
| 7:AI:301:ARG:HB3 | 7:BA:295:ILE:HG13 | 1.88 | 0.54 |
| 7:AJ:463:THR:HG21 | 7:BA:490:ILE:HD12 | 1.88 | 0.54 |
| 1:BI:647:ARG:HD3 | 1:BI:650:TYR:HE2 | 1.71 | 0.54 |
| 2:BJ:153:PHE:O | 2:BJ:154:SER:OG | 2.25 | 0.54 |
| 2:BJ:403:ILE:CG2 | 2:BJ:417:PHE:HB3 | 2.38 | 0.54 |
| 2:BJ:964:PRO:HG2 | 2:BJ:966:PRO:HG3 | 1.89 | 0.54 |
| 2:C:724:ALA:O | 2:C:726:PHE:N | 2.36 | 0.54 |
| 2:C:926:PRO:HD2 | 2:C:985:GLU:O | 2.07 | 0.54 |
| 5:CF:118:LYS:NZ | 5:CF:145:TYR:O | 2.37 | 0.54 |
| 6:CI:13:ARG:NH1 | 6:DA:17:PHE:O | 2.31 | 0.54 |
| 7:DC:295:ILE:HG13 | 7:DD:301:ARG:HB3 | 1.88 | 0.54 |
| 7:DC:429:CYS:HG | 7:DD:515:TRP:HE1 | 1.55 | 0.54 |
| 3:E:46:PRO:HA | 3:E:270:ARG:NH2 | 2.21 | 0.54 |
| 2:EC:775:ASP:O | 2:EC:776:SER:OG | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:794:ASN:HB2 | 2:EC:814:HIS:CE1 | 2.42 | 0.54 |
| 5:EJ:322:GLY:C | 5:EJ:359:GLU:HA | 2.28 | 0.54 |
| 4:F:201:LYS:HB3 | 4:F:280:ALA:HB3 | 1.89 | 0.54 |
| 7:FE:12:GLU:HG3 | 7:FE:14:ARG:H | 1.71 | 0.54 |
| 7:FE:386:ASN:HB2 | 7:FE:387:PRO:HD2 | 1.90 | 0.54 |
| 1:GD:282:GLY:N | 1:GD:312:GLY:O | 2.39 | 0.54 |
| 1:GD:345:TYR:OH | 1:GD:400:ASN:OD1 | 2.25 | 0.54 |
| 1:GD:403:PRO:HG3 | 1:GE:404:ILE:HD12 | 1.90 | 0.54 |
| 2:GF:184:CYS:O | 2:GF:185:LYS:HG2 | 2.07 | 0.54 |
| 2:GF:319:TYR:HD1 | 2:GF:328:TYR:HB2 | 1.71 | 0.54 |
| 2:GF:794:ASN:HB2 | 2:GF:814:HIS:CE1 | 2.42 | 0.54 |
| 4:GI:201:LYS:HB3 | 4:GI:280:ALA:HB3 | 1.90 | 0.54 |
| 5:HC:118:LYS:HA | 5:HC:142:ARG:NH2 | 2.22 | 0.54 |
| 5:HD:275:SER:OG | 5:HD:282:VAL:N | 2.40 | 0.54 |
| 5:HD:289:LYS:HE2 | 5:HD:370:HIS:CE1 | 2.42 | 0.54 |
| 6:HE:135:GLU:HA | 6:HE:138:ALA:HB3 | 1.89 | 0.54 |
| 5:HD:314:ASN:ND2 | 6:HF:8:ALA:O | 2.41 | 0.54 |
| 7:HH:12:GLU:HG3 | 7:HH:14:ARG:H | 1.71 | 0.54 |
| 7:HH:386:ASN:HB2 | 7:HH:387:PRO:HD2 | 1.90 | 0.54 |
| 12:W:228:LEU:HA | 12:IF:19:ASN:OD1 | 2.07 | 0.54 |
| 12:IF:217:THR:O | 12:IF:246:ARG:N | 2.32 | 0.54 |
| 5:J:304:ILE:HG13 | 5:J:386:PHE:H | 1.72 | 0.54 |
| 5:K:39:ASP:HB2 | 5:K:44:TYR:HE2 | 1.72 | 0.54 |
| 6:M:93:THR:HG22 | 6:M:94:VAL:HG23 | 3.79 | 0.54 |
| 7:O:112:ASN:HA | 7:Q:117:THR:OG1 | 2.07 | 0.54 |
| 7:O:325:TYR:HD1 | 7:O:330:ARG:HA | 1.72 | 0.54 |
| 8:R:23:VAL:HA | 8:R:113:VAL:HA | 1.90 | 0.54 |
| 10:U:333:ALA:HA | 12:W:188:LEU:HD23 | 1.89 | 0.54 |
| 1:X:525:ASN:O | 1:X:528:THR:OG1 | 2.11 | 0.54 |
| 1:X:619:GLN:N | 1:X:619:GLN:OE1 | 2.36 | 0.54 |
| 1:X:485:VAL:HG22 | 1:X:624:TYR:HD1 | 1.72 | 0.54 |
| 1:Y:455:PHE:HD2 | 1:Y:456:ASN:HB2 | 1.72 | 0.54 |
| 13:YB:31[F]:VAL:O | 13:YB:35[F]:HIS:HB2 | 2.08 | 0.54 |
| 13:YA:442[F]:THR:HG21 | 13:YB:438[F]:LEU:HD22 | 1.88 | 0.54 |
| 13:YB:474[F]:ILE:HD11 | 13:YC:470[F]:ARG:HD2 | 1.89 | 0.54 |
| 13:YB:61[A]:ILE:HA | 13:YC:76[A]:PRO:C | 2.28 | 0.54 |
| 13:YC:214[B]:MET:HG2 | 13:YC:232[B]:ASN:O | 2.06 | 0.54 |
| 13:YB:498[F]:VAL:HA | 13:YC:490[F]:VAL:O | 2.07 | 0.54 |
| 13:YB:529[A]:THR:N | 13:YC:520[A]:THR:O | 2.41 | 0.54 |
| 13:YB:565[F]:TYR:CZ | 13:YC:557[F]:MET:HG2 | 2.42 | 0.54 |
| 13:YC:26[D]:ARG:HA | 13:YC:55[D]:MET:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:18[A]:ARG:NH1 | 13:YC:77[A]:VAL:HG23 | 2.23 | 0.54 |
| 13:YB:7[F]:ASN:ND2 | 13:YC:9[F]:ASN:HA | 2.14 | 0.54 |
| 14:YD:30[C]:GLU:OE2 | 14:YD:31[C]:LEU:N | 2.40 | 0.54 |
| 14:YD:30[F]:GLU:OE2 | 14:YD:31[F]:LEU:N | 2.40 | 0.54 |
| 14:YE:156[C]:TYR:O | 14:YE:177[C]:ALA:HA | 2.07 | 0.54 |
| 14:YE:30[A]:GLU:OE2 | 14:YE:31[A]:LEU:N | 2.40 | 0.54 |
| 14:YE:30[D]:GLU:OE2 | 14:YE:31[D]:LEU:N | 2.40 | 0.54 |
| 14:YD:238[D]:THR:OG1 | 14:YE:92[D]:HIS:NE2 | 2.40 | 0.54 |
| 14:YE:98[B]:ASP:OD1 | 14:YE:99[B]:SER:N | 2.39 | 0.54 |
| 14:YF:178[E]:LEU:HD11 | 14:YF:183[E]:ASP:HA | 1.89 | 0.54 |
| 14:YF:17[D]:PHE:CD2 | 14:YF:28[D]:PHE:HB3 | 2.43 | 0.54 |
| 14:YF:17[C]:PHE:CD2 | 14:YF:28[C]:PHE:HB3 | 2.43 | 0.54 |
| 14:YF:16[D]:LEU:HA | 14:YF:69[D]:ILE:O | 2.08 | 0.54 |
| 2:Z:148:ASN:HA | 2:Z:168:ILE:HD13 | 1.90 | 0.54 |
| 2:Z:504:GLN:CD | 2:Z:505:PRO:HD2 | 2.27 | 0.54 |
| 2:Z:773:GLN:N | 2:Z:837:GLU:O | 2.33 | 0.54 |
| 5:AC:200:LEU:HG | 5:AC:201:TYR:N | 2.22 | 0.54 |
| 5:AC:339:GLU:HB3 | 6:AG:172:SER:O | 2.08 | 0.54 |
| 5:AE:185:SER:HB2 | 5:AE:228:PHE:HE1 | 1.72 | 0.54 |
| 7:AJ:29:ILE:O | 7:AJ:30:THR:OG1 | 2.24 | 0.54 |
| 7:AJ:63:GLU:O | 7:AJ:67:ILE:HG12 | 2.07 | 0.54 |
| 10:BE:205:LYS:HE2 | 10:BE:207:PHE:HE1 | 1.73 | 0.54 |
| 10:BE:333:ALA:HA | 12:BG:188:LEU:HD23 | 1.89 | 0.54 |
| 1:BH:60:LEU:HD22 | 2:BJ:671:TYR:CD1 | 2.42 | 0.54 |
| 1:BI:544:ASP:OD1 | 1:BI:545:ARG:N | 2.41 | 0.54 |
| 2:BJ:143:MET:HG2 | 2:BJ:544:VAL:HG22 | 1.88 | 0.54 |
| 2:BJ:158:VAL:O | 2:BJ:593:GLU:HA | 2.08 | 0.54 |
| 2:C:191:TYR:HE1 | 2:C:235:LYS:HA | 1.73 | 0.54 |
| 2:C:981:GLN:CG | 2:C:982:LEU:H | 2.19 | 0.54 |
| 3:CA:231:TRP:O | 3:CA:234:ASP:N | 2.39 | 0.54 |
| 3:D:150:LYS:HA | 3:D:160:TRP:CE3 | 2.43 | 0.54 |
| 7:DB:140:GLY:HA2 | 7:DD:129:PHE:HZ | 1.72 | 0.54 |
| 7:DB:386:ASN:HB2 | 7:DB:387:PRO:HD2 | 1.90 | 0.54 |
| 7:DC:211:SER:N | 7:DC:214:THR:OG1 | 2.28 | 0.54 |
| 7:DD:145:SER:O | 7:DD:164:LYS:NZ | 2.25 | 0.54 |
| 7:DD:255:SER:HB3 | 7:DD:263:VAL:HG13 | 1.89 | 0.54 |
| 8:DE:82:ARG:HH12 | 8:DE:138:GLY:HA2 | 1.73 | 0.54 |
| 3:E:254:ASP:OD1 | 3:E:255:SER:N | 2.41 | 0.54 |
| 2:EC:369:ASP:OD1 | 2:EC:436:THR:HG23 | 2.08 | 0.54 |
| 2:EC:790:THR:HA | 3:EE:82:LEU:HD13 | 1.89 | 0.54 |
| 4:EH:111:ASN:OD1 | 4:EH:114:GLY:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:319:GLU:OE2 | 5:EI:324:VAL:HG13 | 2.08 | 0.54 |
| 5:EJ:303:PRO:HB3 | 5:EJ:385:TRP:CZ2 | 2.42 | 0.54 |
| 5:FA:289:LYS:O | 5:FA:290:SER:OG | 2.25 | 0.54 |
| 5:FA:419:ASP:HB3 | 5:FA:436:VAL:HB | 1.89 | 0.54 |
| 6:FC:23:LYS:HB3 | 6:FC:26:ASP:HB2 | 1.88 | 0.54 |
| 7:FG:365:GLY:O | 7:FG:392:LEU:N | 2.25 | 0.54 |
| 7:FG:392:LEU:HD22 | 7:FG:523:ILE:HG21 | 1.89 | 0.54 |
| 8:BC:55:ASN:HB3 | 8:FI:99:ILE:HD11 | 1.88 | 0.54 |
| 1:EA:52:ARG:NH2 | 9:FJ:25:ARG:HB3 | 2.23 | 0.54 |
| 11:GB:142:LYS:HB3 | 11:GB:143:TYR:HD2 | 1.71 | 0.54 |
| 12:DJ:137:TYR:CD2 | 12:GC:221:ILE:HG12 | 2.42 | 0.54 |
| 12:GC:247:VAL:HG12 | 12:GC:248:MET:H | 1.71 | 0.54 |
| 2:GF:148:ASN:HA | 2:GF:168:ILE:HD13 | 1.90 | 0.54 |
| 2:GF:403:ILE:CG2 | 2:GF:417:PHE:HB3 | 2.38 | 0.54 |
| 2:GF:543:LYS:HG2 | 2:GF:575:PHE:CZ | 2.43 | 0.54 |
| 2:GF:964:PRO:HG2 | 2:GF:966:PRO:HG3 | 1.89 | 0.54 |
| 4:GJ:124:ILE:HD12 | 4:GJ:137:LEU:HD23 | 1.90 | 0.54 |
| 5:HC:304:ILE:HG13 | 5:HC:386:PHE:H | 1.72 | 0.54 |
| 6:HE:23:LYS:HB3 | 6:HE:26:ASP:HB2 | 1.89 | 0.54 |
| 7:HH:140:GLY:HA2 | 7:HJ:129:PHE:HZ | 1.70 | 0.54 |
| 10:ID:205:LYS:HE2 | 10:ID:207:PHE:HE1 | 1.73 | 0.54 |
| 12:W:221:ILE:HG12 | 12:IF:137:TYR:CD2 | 2.42 | 0.54 |
| 5:J:290:SER:HA | 5:J:371:PHE:HB3 | 1.88 | 0.54 |
| 5:K:259:THR:OG1 | 5:K:385:TRP:HB2 | 2.07 | 0.54 |
| 7:P:63:GLU:O | 7:P:67:ILE:HG12 | 2.08 | 0.54 |
| 7:O:140:GLY:HA2 | 7:Q:129:PHE:HZ | 1.69 | 0.54 |
| 7:Q:194:ALA:HB2 | 7:Q:208:TYR:HB3 | 1.88 | 0.54 |
| 10:U:205:LYS:HE2 | 10:U:207:PHE:HE1 | 1.73 | 0.54 |
| 10:U:210:ASP:HA | 10:U:343:THR:HG22 | 1.90 | 0.54 |
| 13:YA:31[F]:VAL:O | 13:YA:35[F]:HIS:HB2 | 2.08 | 0.54 |
| 13:YB:26[F]:ARG:HA | 13:YB:55[F]:MET:O | 2.07 | 0.54 |
| 13:YB:565[D]:TYR:CZ | 13:YC:557[D]:MET:HG2 | 2.42 | 0.54 |
| 13:YA:61[C]:ILE:HA | 13:YB:76[C]:PRO:C | 2.26 | 0.54 |
| 13:YB:18[A]:ARG:NH1 | 13:YB:77[A]:VAL:HG23 | 2.23 | 0.54 |
| 13:YB:474[B]:ILE:HD11 | 13:YC:470[B]:ARG:HD2 | 1.89 | 0.54 |
| 13:YB:529[B]:THR:N | 13:YC:520[B]:THR:O | 2.41 | 0.54 |
| 13:YC:82[C]:VAL:HG22 | 13:YC:98[C]:GLY:O | 2.07 | 0.54 |
| 14:YD:178[C]:LEU:HD11 | 14:YD:183[C]:ASP:HA | 1.89 | 0.54 |
| 14:YD:43[D]:SER:OG | 14:YD:45[D]:TYR:N | 2.41 | 0.54 |
| 14:YD:98[D]:ASP:OD1 | 14:YD:99[D]:SER:N | 2.39 | 0.54 |
| 14:YE:178[A]:LEU:HD11 | 14:YE:183[A]:ASP:HA | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:178[E]:LEU:HD11 | 14:YE:183[E]:ASP:HA | 1.89 | 0.54 |
| 14:YE:17[E]:PHE:CD2 | 14:YE:28[E]:PHE:HB3 | 2.43 | 0.54 |
| 14:YE:16[E]:LEU:HA | 14:YE:69[E]:ILE:O | 2.08 | 0.54 |
| 14:YF:123[A]:PRO:HA | 14:YF:161[A]:PRO:HA | 1.90 | 0.54 |
| 14:YF:16[C]:LEU:HA | 14:YF:69[C]:ILE:O | 2.08 | 0.54 |
| 14:YF:43[E]:SER:OG | 14:YF:45[E]:TYR:N | 2.41 | 0.54 |
| 2:Z:153:PHE:O | 2:Z:154:SER:OG | 2.25 | 0.54 |
| 15:ZA:16[B]:ALA:HB3 | 15:ZA:48[B]:GLU:HB2 | 1.90 | 0.54 |
| 15:ZA:2[D]:SER:N | 15:ZA:96[D]:ILE:O | 2.41 | 0.54 |
| 4:AA:124:ILE:HD12 | 4:AA:137:LEU:HD23 | 1.90 | 0.54 |
| 5:AC:319:GLU:OE2 | 5:AC:324:VAL:HG13 | 2.08 | 0.54 |
| 5:AC:146:VAL:HG21 | 5:AD:153:LYS:HD3 | 1.90 | 0.54 |
| 5:AD:180:VAL:HG13 | 5:AD:181:PHE:H | 1.72 | 0.54 |
| 7:AJ:515:TRP:CZ2 | 7:BA:439:ILE:HG23 | 2.42 | 0.54 |
| 8:BB:17:ARG:NH2 | 8:BB:118:ARG:HD3 | 2.23 | 0.54 |
| 8:BC:82:ARG:HH12 | 8:BC:138:GLY:HA2 | 1.73 | 0.54 |
| 1:BH:447:TYR:HB2 | 1:BH:467:TYR:HD2 | 1.73 | 0.54 |
| 2:C:138:ASN:OD1 | 2:C:139:ASN:N | 2.40 | 0.54 |
| 3:CB:254:ASP:OD1 | 3:CB:255:SER:N | 2.41 | 0.54 |
| 4:CE:201:LYS:HB3 | 4:CE:280:ALA:HB3 | 1.90 | 0.54 |
| 5:CH:193:VAL:O | 5:CH:199:GLU:N | 2.38 | 0.54 |
| 5:CH:20:ARG:HH12 | 5:CH:24:ILE:HD12 | 1.73 | 0.54 |
| 5:CH:275:SER:OG | 5:CH:282:VAL:N | 2.40 | 0.54 |
| 5:CH:3:GLN:HG3 | 5:CH:25:LYS:HG3 | 1.88 | 0.54 |
| 5:CH:506:LEU:HB3 | 5:CH:510:GLY:HA2 | 1.89 | 0.54 |
| 5:CH:477:SER:N | 5:CH:602:ALA:O | 2.28 | 0.54 |
| 7:DC:239:ASN:OD1 | 7:DC:253:ARG:NH2 | 2.40 | 0.54 |
| 7:DD:365:GLY:O | 7:DD:392:LEU:N | 2.25 | 0.54 |
| 7:DB:438:GLN:HB2 | 7:DD:516:ASN:OD1 | 2.07 | 0.54 |
| 8:DF:23:VAL:HA | 8:DF:113:VAL:HA | 1.90 | 0.54 |
| 9:DG:53:PHE:HA | 9:DG:84:TYR:HE2 | 1.70 | 0.54 |
| 12:DJ:153:ARG:HH12 | 12:GC:184:PRO:HA | 1.71 | 0.54 |
| 12:DJ:247:VAL:HG12 | 12:DJ:248:MET:H | 1.71 | 0.54 |
| 3:D:313:GLU:HG3 | 3:E:10:ALA:HB2 | 1.89 | 0.54 |
| 1:EB:297:VAL:HG11 | 1:EB:300:ILE:HG23 | 1.90 | 0.54 |
| 1:EB:544:ASP:OD1 | 1:EB:545:ARG:N | 2.41 | 0.54 |
| 2:EC:180:ILE:HA | 2:EC:219:TRP:HH2 | 1.73 | 0.54 |
| 2:EC:403:ILE:CG2 | 2:EC:417:PHE:HB3 | 2.38 | 0.54 |
| 2:EC:901:ASN:OD1 | 3:EE:333:THR:OG1 | 2.23 | 0.54 |
| 4:EH:124:ILE:HD12 | 4:EH:137:LEU:HD23 | 1.90 | 0.54 |
| 5:EJ:256:SER:HB2 | 5:EJ:387:ASN:OD1 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FD:23:LYS:HB3 | 6:FD:26:ASP:HB2 | 1.88 | 0.54 |
| 7:FF:36:ILE:HG13 | 7:FG:18:PHE:HE1 | 1.73 | 0.54 |
| 7:FF:93:THR:HG22 | 7:FF:94:VAL:HG23 | 1.89 | 0.54 |
| 9:FJ:53:PHE:HA | 9:FJ:84:TYR:HE2 | 1.70 | 0.54 |
| 1:GD:307:ASP:HB3 | 1:GD:309:ASP:N | 2.22 | 0.54 |
| 1:GE:196:GLN:HG3 | 1:GE:273:ILE:HD12 | 1.88 | 0.54 |
| 2:GF:450:PHE:CD1 | 2:GF:453:ASP:HB2 | 2.43 | 0.54 |
| 2:GF:653:MET:HB3 | 2:GF:658:LEU:HD11 | 1.89 | 0.54 |
| 4:GJ:201:LYS:HB3 | 4:GJ:280:ALA:HB3 | 1.90 | 0.54 |
| 4:HA:111:ASN:OD1 | 4:HA:114:GLY:N | 2.41 | 0.54 |
| 4:HA:154:ASP:HB2 | 4:HA:157:THR:HB | 1.88 | 0.54 |
| 6:HF:23:LYS:HB3 | 6:HF:26:ASP:HB2 | 1.88 | 0.54 |
| 7:HI:239:ASN:OD1 | 7:HI:253:ARG:NH2 | 2.40 | 0.54 |
| 7:HJ:418:ASP:OD1 | 7:HJ:422:LYS:N | 2.28 | 0.54 |
| 8:FH:117:ALA:HA | 8:IA:77:GLU:OE2 | 2.08 | 0.54 |
| 10:ID:210:ASP:HA | 10:ID:343:THR:HG22 | 1.90 | 0.54 |
| 11:IE:133:TRP:CZ2 | 11:IE:150:LEU:HD11 | 2.42 | 0.54 |
| 5:J:330:HIS:ND1 | 5:J:355:ASP:HB2 | 2.23 | 0.54 |
| 5:K:118:LYS:HA | 5:K:142:ARG:NH2 | 2.23 | 0.54 |
| 5:K:20:ARG:HH12 | 5:K:24:ILE:HD12 | 1.73 | 0.54 |
| 7:O:118:PRO:HG3 | 7:P:106:ALA:HA | 1.90 | 0.54 |
| 7:P:93:THR:HG22 | 7:P:94:VAL:HG23 | 1.89 | 0.54 |
| 10:U:212:THR:HG21 | 12:IF:149:ARG:HB3 | 1.88 | 0.54 |
| 10:U:286:VAL:HG22 | 10:U:287:VAL:H | 1.73 | 0.54 |
| 1:Y:213:SER:OG | 1:Y:337:GLN:OE1 | 2.23 | 0.54 |
| 13:YB:214[D]:MET:HG2 | 13:YB:232[D]:ASN:O | 2.06 | 0.54 |
| 13:YB:437[B]:ASN:HB3 | 13:YB:439[B]:TYR:CE1 | 2.43 | 0.54 |
| 13:YA:503[D]:THR:O | 13:YB:495[D]:THR:HA | 2.06 | 0.54 |
| 13:YC:425[F]:SER:HB2 | 13:YC:426[F]:PRO:HD2 | 1.89 | 0.54 |
| 13:YB:498[A]:VAL:HA | 13:YC:490[A]:VAL:O | 2.07 | 0.54 |
| 13:YA:519[B]:THR:HA | 13:YC:527[B]:THR:O | 2.07 | 0.54 |
| 13:YC:26[F]:ARG:HA | 13:YC:55[F]:MET:O | 2.07 | 0.54 |
| 14:YD:123[F]:PRO:HA | 14:YD:161[F]:PRO:HA | 1.90 | 0.54 |
| 13:YA:90[E]:TRP:NE1 | 14:YD:175[E]:GLU:OE1 | 2.36 | 0.54 |
| 14:YD:43[E]:SER:OG | 14:YD:45[E]:TYR:N | 2.41 | 0.54 |
| 14:YE:17[D]:PHE:CD2 | 14:YE:28[D]:PHE:HB3 | 2.43 | 0.54 |
| 14:YE:189[F]:TRP:NE1 | 14:YE:320[F]:PRO:HG2 | 2.21 | 0.54 |
| 14:YE:43[A]:SER:OG | 14:YE:45[A]:TYR:N | 2.41 | 0.54 |
| 10:GA:285:LEU:HA | 14:YF:215[A]:GLU:CG | 2.38 | 0.54 |
| 14:YF:30[E]:GLU:OE2 | 14:YF:31[E]:LEU:N | 2.40 | 0.54 |
| 2:Z:101:GLU:OE1 | 2:Z:101:GLU:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:127:PHE:O | 2:Z:130:ASN:N | 2.41 | 0.54 |
| 2:Z:422:GLU:HB3 | 2:Z:423:GLU:OE1 | 2.06 | 0.54 |
| 2:Z:437:ASP:HA | 2:Z:516:TRP:CE3 | 2.42 | 0.54 |
| 15:ZA:16[A]:ALA:HB3 | 15:ZA:48[A]:GLU:HB2 | 1.89 | 0.54 |
| 1:A:307:ASP:HB3 | 1:A:309:ASP:N | 2.22 | 0.54 |
| 5:AC:419:ASP:HB3 | 5:AC:436:VAL:HB | 1.88 | 0.54 |
| 5:AE:3:GLN:HG3 | 5:AE:25:LYS:HG3 | 1.88 | 0.54 |
| 5:AE:359:GLU:O | 5:AE:370:HIS:N | 2.36 | 0.54 |
| 5:AE:357:SER:OG | 6:AG:4:LEU:HD21 | 2.08 | 0.54 |
| 1:A:403:PRO:HG3 | 1:B:404:ILE:HD12 | 1.90 | 0.54 |
| 7:BA:176:ILE:HG23 | 7:BA:177:ALA:H | 1.73 | 0.54 |
| 7:AI:449:GLY:N | 7:BA:482:TYR:O | 2.32 | 0.54 |
| 8:BB:23:VAL:HA | 8:BB:113:VAL:HA | 1.90 | 0.54 |
| 8:BB:55:ASN:HB3 | 8:FH:99:ILE:HD11 | 1.90 | 0.54 |
| 8:BC:130:LYS:NZ | 8:BC:163:GLU:OE2 | 2.37 | 0.54 |
| 1:BH:345:TYR:OH | 1:BH:400:ASN:OD1 | 2.25 | 0.54 |
| 1:BI:297:VAL:HG11 | 1:BI:300:ILE:HG23 | 1.90 | 0.54 |
| 2:BJ:148:ASN:HA | 2:BJ:168:ILE:HD13 | 1.90 | 0.54 |
| 2:BJ:900:ILE:HG13 | 3:CB:311:TYR:CE1 | 2.43 | 0.54 |
| 2:C:422:GLU:HB3 | 2:C:423:GLU:OE1 | 2.06 | 0.54 |
| 2:C:504:GLN:CD | 2:C:505:PRO:HD2 | 2.27 | 0.54 |
| 4:CD:111:ASN:OD1 | 4:CD:114:GLY:N | 2.41 | 0.54 |
| 4:CD:124:ILE:HD12 | 4:CD:137:LEU:HD23 | 1.90 | 0.54 |
| 4:CE:124:ILE:HD12 | 4:CE:137:LEU:HD23 | 1.90 | 0.54 |
| 5:CG:13:ASP:OD1 | 5:CG:14:GLY:N | 2.41 | 0.54 |
| 5:CH:415:ASP:HB2 | 5:CH:440:GLN:HE22 | 1.71 | 0.54 |
| 7:DB:325:TYR:HD1 | 7:DB:330:ARG:HA | 1.72 | 0.54 |
| 7:DC:463:THR:HG21 | 7:DD:490:ILE:HD12 | 1.88 | 0.54 |
| 1:EA:522:LYS:HB3 | 1:EA:533:ASP:HA | 1.89 | 0.54 |
| 2:EC:450:PHE:CD1 | 2:EC:453:ASP:HB2 | 2.43 | 0.54 |
| 3:EE:150:LYS:HA | 3:EE:160:TRP:CE3 | 2.42 | 0.54 |
| 5:EI:265:LEU:HG | 5:EI:379:ASP:HB2 | 1.90 | 0.54 |
| 5:EI:594:THR:OG1 | 5:EJ:517:GLY:N | 2.41 | 0.54 |
| 5:EJ:396:LYS:O | 5:EJ:399:ILE:HG13 | 2.08 | 0.54 |
| 5:EI:484:GLY:N | 5:EJ:489:GLY:O | 2.32 | 0.54 |
| 7:FE:438:GLN:HB2 | 7:FG:516:ASN:OD1 | 2.07 | 0.54 |
| 4:G:154:ASP:HB2 | 4:G:157:THR:HB | 1.88 | 0.54 |
| 10:GA:210:ASP:HA | 10:GA:343:THR:HG22 | 1.90 | 0.54 |
| 1:GE:189:ASP:HA | 11:IE:121:TYR:HE2 | 1.73 | 0.54 |
| 2:GF:180:ILE:HA | 2:GF:219:TRP:HH2 | 1.73 | 0.54 |
| 3:GG:150:LYS:HA | 3:GG:160:TRP:CE3 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:HA:201:LYS:HB3 | 4:HA:280:ALA:HB3 | 1.90 | 0.54 |
| 5:HB:103:ASN:OD1 | 5:HB:104:VAL:N | 2.39 | 0.54 |
| 5:HB:372:ASP:N | 5:HB:372:ASP:OD1 | 2.40 | 0.54 |
| 5:HB:399:ILE:HG23 | 5:HD:399:ILE:HD13 | 1.89 | 0.54 |
| 5:HC:204:ASP:OD1 | 5:HC:205:VAL:N | 2.41 | 0.54 |
| 5:HC:36:GLU:HA | 5:HC:50:LYS:NZ | 2.22 | 0.54 |
| 5:HD:118:LYS:HA | 5:HD:142:ARG:NH2 | 2.23 | 0.54 |
| 7:Q:149:GLN:OE1 | 6:HE:184:SER:HA | 2.08 | 0.54 |
| 7:HJ:354:LEU:HG | 7:HJ:361:PHE:CZ | 2.42 | 0.54 |
| 7:HI:463:THR:HG21 | 7:HJ:490:ILE:HD12 | 1.88 | 0.54 |
| 5:J:94:ARG:HD3 | 5:J:134:GLU:HG2 | 1.89 | 0.54 |
| 1:Y:90:VAL:HG13 | 1:Y:100:PRO:HG3 | 1.87 | 0.54 |
| 1:Y:510:MET:HB3 | 1:Y:542:SER:HB3 | 1.89 | 0.54 |
| 13:YA:437[D]:ASN:HB3 | 13:YA:439[D]:TYR:CE1 | 2.43 | 0.54 |
| 13:YA:26[A]:ARG:HA | 13:YA:55[A]:MET:O | 2.07 | 0.54 |
| 13:YB:437[D]:ASN:HB3 | 13:YB:439[D]:TYR:CE1 | 2.43 | 0.54 |
| 13:YB:522[E]:VAL:HG23 | 13:YC:516[E]:GLY:O | 2.08 | 0.54 |
| 13:YB:522[F]:VAL:HG23 | 13:YC:516[F]:GLY:O | 2.08 | 0.54 |
| 1:X:526:PRO:HB3 | 13:YC:254[F]:ARG:HD3 | 1.89 | 0.54 |
| 13:YC:437[A]:ASN:HB3 | 13:YC:439[A]:TYR:CE1 | 2.43 | 0.54 |
| 14:YD:50[D]:GLY:O | 14:YD:109[D]:LEU:N | 2.38 | 0.54 |
| 14:YD:123[E]:PRO:HA | 14:YD:161[E]:PRO:HA | 1.90 | 0.54 |
| 14:YD:178[A]:LEU:HD11 | 14:YD:183[A]:ASP:HA | 1.89 | 0.54 |
| 14:YD:17[A]:PHE:CD2 | 14:YD:28[A]:PHE:HB3 | 2.43 | 0.54 |
| 10:BE:285:LEU:HA | 14:YE:215[A]:GLU:CG | 2.38 | 0.54 |
| 14:YE:43[F]:SER:OG | 14:YE:45[F]:TYR:N | 2.40 | 0.54 |
| 14:YE:238[A]:THR:OG1 | 14:YF:92[A]:HIS:NE2 | 2.40 | 0.54 |
| 2:Z:158:VAL:O | 2:Z:593:GLU:HA | 2.08 | 0.54 |
| 2:Z:177:GLN:HG3 | 2:Z:215:LYS:HB2 | 1.90 | 0.54 |
| 1:A:554:ILE:HG21 | 1:A:577:PHE:CD1 | 2.43 | 0.54 |
| 4:AA:111:ASN:OD1 | 4:AA:114:GLY:N | 2.41 | 0.54 |
| 5:AD:118:LYS:HA | 5:AD:142:ARG:NH2 | 2.22 | 0.54 |
| 5:AD:13:ASP:OD1 | 5:AD:14:GLY:N | 2.41 | 0.54 |
| 5:AE:180:VAL:HG13 | 5:AE:181:PHE:H | 1.73 | 0.54 |
| 6:AF:23:LYS:HB3 | 6:AF:26:ASP:HB2 | 1.88 | 0.54 |
| 7:AI:322:THR:HG23 | 7:AJ:327:GLN:HE21 | 1.73 | 0.54 |
| 7:AI:325:TYR:HD1 | 7:AI:330:ARG:HA | 1.72 | 0.54 |
| 7:AJ:440:GLN:OE1 | 7:AJ:511:GLU:HG3 | 2.08 | 0.54 |
| 1:B:544:ASP:OD1 | 1:B:545:ARG:N | 2.41 | 0.54 |
| 7:AJ:518:SER:HB3 | 7:BA:403:SER:HA | 1.90 | 0.54 |
| 1:BI:102:SER:H | 1:BI:194:ARG:NH1 | 2.02 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:287:LEU:HD12 | 2:BJ:289:PHE:H | 1.73 | 0.54 |
| 2:BJ:351:GLU:CB | 2:BJ:353:ASP:HB2 | 2.31 | 0.54 |
| 2:BJ:369:ASP:OD1 | 2:BJ:436:THR:HG23 | 2.08 | 0.54 |
| 2:BJ:543:LYS:HG2 | 2:BJ:575:PHE:CZ | 2.43 | 0.54 |
| 2:BJ:947:VAL:O | 3:CA:117:ALA:HB1 | 2.08 | 0.54 |
| 2:C:316:ASP:O | 2:C:331:THR:N | 2.34 | 0.54 |
| 2:C:543:LYS:HG2 | 2:C:575:PHE:CZ | 2.43 | 0.54 |
| 3:CB:197:ASP:N | 3:CB:197:ASP:OD1 | 2.38 | 0.54 |
| 4:CE:111:ASN:OD1 | 4:CE:114:GLY:N | 2.41 | 0.54 |
| 5:CG:303:PRO:HB3 | 5:CG:385:TRP:CZ2 | 2.42 | 0.54 |
| 5:CH:118:LYS:HA | 5:CH:142:ARG:NH2 | 2.23 | 0.54 |
| 3:D:74:HIS:NE2 | 2:GF:449:LYS:HD2 | 2.23 | 0.54 |
| 7:DC:63:GLU:O | 7:DC:67:ILE:HG12 | 2.08 | 0.54 |
| 7:DB:199:VAL:HG12 | 7:DD:212:PRO:HG3 | 1.89 | 0.54 |
| 7:DD:85:LEU:O | 7:DD:86:SER:OG | 2.21 | 0.54 |
| 8:DE:23:VAL:HA | 8:DE:113:VAL:HA | 1.90 | 0.54 |
| 8:DF:17:ARG:NH2 | 8:DF:118:ARG:HD3 | 2.23 | 0.54 |
| 11:DI:54:PRO:HG2 | 11:DI:59:LEU:HB2 | 1.90 | 0.54 |
| 1:EB:510:MET:HB3 | 1:EB:542:SER:HB3 | 1.89 | 0.54 |
| 2:EC:174:HIS:CG | 2:EC:508:TYR:HH | 2.25 | 0.54 |
| 4:EF:111:ASN:HD21 | 4:EF:116:ILE:H | 1.56 | 0.54 |
| 4:EF:172:GLU:HA | 4:EG:166:SER:H | 1.72 | 0.54 |
| 5:EI:36:GLU:HA | 5:EI:50:LYS:HZ1 | 1.71 | 0.54 |
| 5:EJ:13:ASP:OD1 | 5:EJ:14:GLY:N | 2.41 | 0.54 |
| 5:EJ:137:TYR:HA | 5:EJ:143:TRP:HD1 | 1.73 | 0.54 |
| 5:EJ:330:HIS:ND1 | 5:EJ:355:ASP:HB2 | 2.23 | 0.54 |
| 5:EI:194:LYS:HE3 | 5:FA:198:ASN:HD22 | 1.73 | 0.54 |
| 5:EJ:465:ASN:ND2 | 5:FA:418:GLY:O | 2.41 | 0.54 |
| 6:FB:23:LYS:HB3 | 6:FB:26:ASP:HB2 | 1.89 | 0.54 |
| 7:FF:134:SER:HB3 | 7:FF:140:GLY:N | 2.23 | 0.54 |
| 9:FJ:62:PHE:HE2 | 9:FJ:129:SER:H | 1.56 | 0.54 |
| 1:GE:455:PHE:HD2 | 1:GE:456:ASN:HB2 | 1.72 | 0.54 |
| 2:GF:158:VAL:O | 2:GF:593:GLU:HA | 2.08 | 0.54 |
| 2:GF:39:ALA:HB1 | 2:GF:54:TYR:CE1 | 2.42 | 0.54 |
| 2:GF:947:VAL:O | 3:GG:117:ALA:HB1 | 2.07 | 0.54 |
| 3:GH:150:LYS:HA | 3:GH:160:TRP:CE3 | 2.42 | 0.54 |
| 4:F:4:GLN:NE2 | 4:H:61:ILE:O | 2.39 | 0.54 |
| 5:HB:520:GLY:O | 5:HD:591:PRO:HA | 2.08 | 0.54 |
| 5:HC:322:GLY:C | 5:HC:359:GLU:HA | 2.28 | 0.54 |
| 7:HI:296:ILE:HG22 | 7:HI:298:GLY:H | 1.73 | 0.54 |
| 7:HI:32:VAL:O | 7:HI:36:ILE:HG12 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:63:GLU:O | 7:HI:67:ILE:HG12 | 2.08 | 0.54 |
| 7:HJ:233:GLN:HE21 | 7:HJ:237:ASN:HD21 | 1.56 | 0.54 |
| 5:I:419:ASP:HB3 | 5:I:436:VAL:HB | 1.88 | 0.54 |
| 12:GC:153:ARG:HH12 | 12:IF:184:PRO:HA | 1.71 | 0.54 |
| 5:J:180:VAL:HG13 | 5:J:181:PHE:H | 1.73 | 0.54 |
| 6:M:69:THR:HA | 6:N:73:ASN:HB3 | 1.90 | 0.54 |
| 7:O:447:HIS:CD2 | 7:Q:447:HIS:HD2 | 2.25 | 0.54 |
| 7:P:263:VAL:O | 7:Q:255:SER:OG | 2.14 | 0.54 |
| 8:S:23:VAL:HA | 8:S:113:VAL:HA | 1.90 | 0.54 |
| 8:S:17:ARG:NH2 | 8:S:118:ARG:HD3 | 2.23 | 0.54 |
| 1:X:8:TYR:CZ | 1:X:20:ILE:HG22 | 2.42 | 0.54 |
| 13:YA:495[C]:THR:HA | 13:YC:503[C]:THR:O | 2.08 | 0.54 |
| 13:YA:76[C]:PRO:C | 13:YC:61[C]:ILE:HA | 2.29 | 0.54 |
| 13:YA:57[F]:VAL:CB | 13:YA:76[F]:PRO:HD3 | 2.37 | 0.54 |
| 13:YB:498[B]:VAL:HA | 13:YC:490[B]:VAL:O | 2.07 | 0.54 |
| 13:YB:565[C]:TYR:CZ | 13:YC:557[C]:MET:HG2 | 2.42 | 0.54 |
| 13:YB:18[C]:ARG:NH1 | 13:YB:77[C]:VAL:HG23 | 2.23 | 0.54 |
| 13:YC:437[B]:ASN:HB3 | 13:YC:439[B]:TYR:CE1 | 2.43 | 0.54 |
| 13:YA:466[A]:ASN:HB2 | 13:YC:474[A]:ILE:HG12 | 1.89 | 0.54 |
| 14:YD:17[C]:PHE:CD2 | 14:YD:28[C]:PHE:HB3 | 2.43 | 0.54 |
| 14:YD:16[A]:LEU:HA | 14:YD:69[A]:ILE:O | 2.08 | 0.54 |
| 14:YD:16[B]:LEU:HA | 14:YD:69[B]:ILE:O | 2.08 | 0.54 |
| 14:YE:178[D]:LEU:HD11 | 14:YE:183[D]:ASP:HA | 1.88 | 0.54 |
| 14:YE:17[F]:PHE:CD2 | 14:YE:28[F]:PHE:HB3 | 2.43 | 0.54 |
| 14:YE:16[D]:LEU:HA | 14:YE:69[D]:ILE:O | 2.08 | 0.54 |
| 13:YC:90[C]:TRP:NE1 | 14:YF:175[C]:GLU:OE1 | 2.36 | 0.54 |
| 14:YF:43[A]:SER:OG | 14:YF:45[A]:TYR:N | 2.41 | 0.54 |
| 2:Z:138:ASN:OD1 | 2:Z:139:ASN:N | 2.40 | 0.54 |
| 2:Z:403:ILE:CG2 | 2:Z:417:PHE:HB3 | 2.38 | 0.54 |
| 2:Z:548:ILE:HB | 2:Z:555:ARG:HB3 | 1.89 | 0.54 |
| 2:Z:543:LYS:HG2 | 2:Z:575:PHE:CZ | 2.43 | 0.54 |
| 15:ZA:16[E]:ALA:HB3 | 15:ZA:48[E]:GLU:HB2 | 1.90 | 0.54 |
| 15:ZA:76[F]:GLN:HB3 | 15:ZA:96[F]:ILE:HD11 | 1.90 | 0.54 |
| 5:AC:358:VAL:HG22 | 5:AC:371:PHE:HB2 | 1.88 | 0.54 |
| 6:AG:135:GLU:HA | 6:AG:138:ALA:HB3 | 1.89 | 0.54 |
| 7:AI:231:GLY:HA2 | 7:AJ:222:GLU:HG3 | 1.90 | 0.54 |
| 7:AJ:296:ILE:HG22 | 7:AJ:298:GLY:H | 1.73 | 0.54 |
| 7:BA:211:SER:N | 7:BA:214:THR:OG1 | 2.39 | 0.54 |
| 7:BA:354:LEU:HG | 7:BA:361:PHE:CZ | 2.42 | 0.54 |
| 1:BH:485:VAL:HG22 | 1:BH:624:TYR:HD1 | 1.72 | 0.54 |
| 2:BJ:177:GLN:HG3 | 2:BJ:215:LYS:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:653:MET:HB3 | 2:BJ:658:LEU:HD11 | 1.89 | 0.54 |
| 2:C:228:ARG:HD2 | 5:K:556:GLN:HE22 | 1.73 | 0.54 |
| 2:C:207:PRO:HA | 2:C:229:VAL:HG23 | 1.90 | 0.54 |
| 2:C:450:PHE:CD1 | 2:C:453:ASP:HB2 | 2.43 | 0.54 |
| 2:C:39:ALA:HB1 | 2:C:54:TYR:CE1 | 2.42 | 0.54 |
| 5:CF:94:ARG:CD | 5:CF:134:GLU:HG2 | 2.38 | 0.54 |
| 5:CF:201:TYR:HB3 | 5:CG:166:GLU:HG2 | 1.89 | 0.54 |
| 5:CH:180:VAL:HG13 | 5:CH:181:PHE:H | 1.73 | 0.54 |
| 6:CI:140:PHE:CZ | 7:FF:196:VAL:HG11 | 2.42 | 0.54 |
| 6:DA:23:LYS:HB3 | 6:DA:26:ASP:HB2 | 1.89 | 0.54 |
| 7:DB:100:TYR:OH | 7:DC:113:GLU:HG3 | 2.08 | 0.54 |
| 7:DC:32:VAL:O | 7:DC:36:ILE:HG12 | 2.08 | 0.54 |
| 1:EA:447:TYR:HB2 | 1:EA:467:TYR:HD2 | 1.73 | 0.54 |
| 1:EA:403:PRO:HG3 | 1:EB:404:ILE:HD12 | 1.89 | 0.54 |
| 2:EC:287:LEU:HD12 | 2:EC:289:PHE:H | 1.73 | 0.54 |
| 2:BJ:484:HIS:ND1 | 3:EE:232:GLN:OE1 | 2.32 | 0.54 |
| 5:EI:372:ASP:N | 5:EI:372:ASP:OD1 | 2.40 | 0.54 |
| 5:EJ:261:ARG:NE | 5:EJ:297:GLY:O | 2.30 | 0.54 |
| 5:FA:506:LEU:HB3 | 5:FA:510:GLY:HA2 | 1.89 | 0.54 |
| 5:FA:477:SER:N | 5:FA:602:ALA:O | 2.28 | 0.54 |
| 5:EJ:318:GLN:HB3 | 6:FB:4:LEU:HG | 1.90 | 0.54 |
| 7:FE:447:HIS:CD2 | 7:FG:447:HIS:HD2 | 2.26 | 0.54 |
| 7:FF:447:HIS:HD2 | 7:FG:447:HIS:CD2 | 2.25 | 0.54 |
| 7:FF:429:CYS:HG | 7:FG:515:TRP:HE1 | 1.56 | 0.54 |
| 8:FI:17:ARG:NH2 | 8:FI:118:ARG:HD3 | 2.23 | 0.54 |
| 12:GC:137:TYR:CD2 | 12:IF:221:ILE:HG12 | 2.43 | 0.54 |
| 1:GE:69:GLN:OE1 | 11:IE:70:TYR:HE1 | 1.91 | 0.54 |
| 2:GF:191:TYR:HE1 | 2:GF:235:LYS:HA | 1.73 | 0.54 |
| 2:GF:479:TRP:CD2 | 2:GF:505:PRO:HA | 2.43 | 0.54 |
| 2:GF:504:GLN:CD | 2:GF:505:PRO:HD2 | 2.27 | 0.54 |
| 2:GF:794:ASN:HB2 | 2:GF:814:HIS:NE2 | 2.22 | 0.54 |
| 4:HA:111:ASN:HD21 | 4:HA:116:ILE:H | 1.56 | 0.54 |
| 4:HA:131:LYS:N | 4:HA:160:TRP:O | 2.29 | 0.54 |
| 5:HB:569:TYR:CE2 | 5:HD:542:LEU:HD11 | 2.43 | 0.54 |
| 5:HC:102:TRP:CE3 | 5:HC:131:SER:HB2 | 2.42 | 0.54 |
| 2:GF:221:ALA:N | 5:HC:562:SER:OG | 2.40 | 0.54 |
| 5:HD:264:ARG:HG3 | 5:HD:379:ASP:O | 2.07 | 0.54 |
| 7:HH:213:TYR:HB2 | 7:HI:203:THR:O | 2.08 | 0.54 |
| 7:HI:118:PRO:O | 7:HI:122:THR:N | 2.36 | 0.54 |
| 7:HI:134:SER:HB3 | 7:HI:140:GLY:N | 2.23 | 0.54 |
| 7:HI:289:GLN:OE1 | 7:HI:294:GLN:NE2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:117:ILE:HG13 | 5:I:118:LYS:H | 1.73 | 0.54 |
| 7:Q:20:PRO:HG3 | 7:Q:29:ILE:HG13 | 1.89 | 0.54 |
| 7:Q:457:LEU:HD23 | 7:Q:477:TRP:CZ2 | 2.44 | 0.54 |
| 1:X:187:ILE:HD11 | 1:X:270:ILE:HD13 | 1.91 | 0.54 |
| 1:Y:83:ALA:O | 1:Y:326:ARG:NH2 | 2.36 | 0.54 |
| 13:YA:31[A]:VAL:O | 13:YA:35[A]:HIS:HB2 | 2.08 | 0.54 |
| 13:YA:425[B]:SER:HB2 | 13:YA:426[B]:PRO:HD2 | 1.89 | 0.54 |
| 13:YA:425[D]:SER:HB2 | 13:YA:426[D]:PRO:HD2 | 1.89 | 0.54 |
| 13:YA:71[E]:GLY:HA2 | 13:YB:393[E]:MET:HA | 1.90 | 0.54 |
| 13:YB:425[F]:SER:HB2 | 13:YB:426[F]:PRO:HD2 | 1.89 | 0.54 |
| 13:YA:454[F]:LYS:NZ | 13:YB:464[F]:TYR:OH | 2.41 | 0.54 |
| 13:YB:529[F]:THR:N | 13:YC:520[F]:THR:O | 2.41 | 0.54 |
| 13:YB:538[C]:VAL:HG11 | 13:YC:534[C]:LEU:CB | 2.38 | 0.54 |
| 13:YB:18[D]:ARG:NH1 | 13:YB:77[D]:VAL:HG23 | 2.23 | 0.54 |
| 13:YC:425[D]:SER:HB2 | 13:YC:426[D]:PRO:HD2 | 1.89 | 0.54 |
| 13:YA:495[B]:THR:HA | 13:YC:503[B]:THR:O | 2.08 | 0.54 |
| 14:YD:17[F]:PHE:CD2 | 14:YD:28[F]:PHE:HB3 | 2.43 | 0.54 |
| 14:YE:123[C]:PRO:HA | 14:YE:161[C]:PRO:HA | 1.90 | 0.54 |
| 14:YE:16[F]:LEU:HA | 14:YE:69[F]:ILE:O | 2.08 | 0.54 |
| 14:YE:43[B]:SER:OG | 14:YE:45[B]:TYR:N | 2.41 | 0.54 |
| 14:YE:43[E]:SER:OG | 14:YE:45[E]:TYR:N | 2.41 | 0.54 |
| 14:YF:123[F]:PRO:HA | 14:YF:161[F]:PRO:HA | 1.90 | 0.54 |
| 14:YF:178[B]:LEU:HD11 | 14:YF:183[B]:ASP:HA | 1.88 | 0.54 |
| 14:YF:178[C]:LEU:HD11 | 14:YF:183[C]:ASP:HA | 1.89 | 0.54 |
| 14:YF:178[D]:LEU:HD11 | 14:YF:183[D]:ASP:HA | 1.88 | 0.54 |
| 14:YF:17[E]:PHE:CD2 | 14:YF:28[E]:PHE:HB3 | 2.43 | 0.54 |
| 14:YD:92[C]:HIS:NE2 | 14:YF:238[C]:THR:OG1 | 2.41 | 0.54 |
| 14:YF:50[F]:GLY:O | 14:YF:109[F]:LEU:N | 2.38 | 0.54 |
| 2:Z:205:TYR:HB2 | 2:Z:206:GLN:OE1 | 2.08 | 0.54 |
| 2:Z:39:ALA:HB1 | 2:Z:54:TYR:CE1 | 2.42 | 0.54 |
| 15:ZA:2[B]:SER:N | 15:ZA:96[B]:ILE:O | 2.41 | 0.54 |
| 15:ZA:2[E]:SER:N | 15:ZA:96[E]:ILE:O | 2.41 | 0.54 |
| 1:A:485:VAL:HG22 | 1:A:624:TYR:HD1 | 1.72 | 0.53 |
| 5:AD:396:LYS:O | 5:AD:399:ILE:HG13 | 2.08 | 0.53 |
| 7:AI:110:VAL:HG12 | 7:AI:111:ASN:H | 1.73 | 0.53 |
| 7:AI:112:ASN:HA | 7:BA:117:THR:OG1 | 2.07 | 0.53 |
| 7:AI:447:HIS:CD2 | 7:BA:447:HIS:HD2 | 2.26 | 0.53 |
| 7:AJ:341:ILE:HG13 | 7:BA:341:ILE:HD11 | 1.90 | 0.53 |
| 7:AI:447:HIS:CD2 | 7:AJ:447:HIS:CD2 | 2.95 | 0.53 |
| 7:AJ:476:ASP:CG | 7:AJ:479:ASN:HD21 | 2.09 | 0.53 |
| 11:BF:54:PRO:HG2 | 11:BF:59:LEU:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:307:ASP:HB3 | 1:BH:309:ASP:N | 2.22 | 0.53 |
| 1:BH:45:ASP:OD1 | 1:BH:46:TYR:N | 2.41 | 0.53 |
| 1:BH:642:PHE:CZ | 1:BH:644:ASN:HB2 | 2.44 | 0.53 |
| 1:BI:45:ASP:C | 1:BI:47:ASP:H | 2.10 | 0.53 |
| 2:C:548:ILE:HB | 2:C:555:ARG:HB3 | 1.89 | 0.53 |
| 4:CC:111:ASN:HD21 | 4:CC:116:ILE:H | 1.56 | 0.53 |
| 5:CF:200:LEU:HG | 5:CF:201:TYR:N | 2.22 | 0.53 |
| 5:CG:117:ILE:HG22 | 5:CG:143:TRP:CE3 | 2.42 | 0.53 |
| 5:CH:127:ASN:HD21 | 5:CH:182:ARG:HH12 | 1.56 | 0.53 |
| 7:DB:213:TYR:HB2 | 7:DC:203:THR:O | 2.08 | 0.53 |
| 8:DE:9:ALA:HB2 | 8:FH:34:PHE:HD2 | 1.73 | 0.53 |
| 12:DJ:251:GLY:HA3 | 12:GC:104:PHE:CG | 2.43 | 0.53 |
| 1:EB:67:ILE:HA | 1:EB:70:PHE:HB3 | 1.90 | 0.53 |
| 2:EC:517:SER:O | 2:EC:521:ASN:HA | 2.07 | 0.53 |
| 2:EC:964:PRO:HG2 | 2:EC:966:PRO:HG3 | 1.89 | 0.53 |
| 2:EC:947:VAL:O | 3:ED:117:ALA:HB1 | 2.07 | 0.53 |
| 5:FA:127:ASN:HD21 | 5:FA:182:ARG:HH12 | 1.56 | 0.53 |
| 5:FA:206:PHE:CZ | 5:FA:221:GLU:HG2 | 2.42 | 0.53 |
| 7:FF:32:VAL:O | 7:FF:36:ILE:HG12 | 2.08 | 0.53 |
| 7:FF:384:GLY:O | 7:FF:391:GLY:N | 2.36 | 0.53 |
| 7:FG:372:CYS:SG | 7:FG:525:VAL:HB | 2.49 | 0.53 |
| 8:FH:115:GLN:HG2 | 8:IA:79:HIS:HE2 | 1.74 | 0.53 |
| 8:DF:43:ALA:HB2 | 8:FI:139:GLU:H | 1.72 | 0.53 |
| 11:GB:31:ASN:OD1 | 11:GB:32:TYR:N | 2.41 | 0.53 |
| 1:GD:423:THR:O | 1:GD:476:ILE:N | 2.35 | 0.53 |
| 2:GF:101:GLU:N | 2:GF:101:GLU:OE1 | 2.41 | 0.53 |
| 2:GF:287:LEU:HD12 | 2:GF:289:PHE:H | 1.73 | 0.53 |
| 4:GI:111:ASN:HD21 | 4:GI:116:ILE:H | 1.56 | 0.53 |
| 4:H:161:ASN:OD1 | 4:H:162:TYR:N | 2.41 | 0.53 |
| 5:HD:206:PHE:CZ | 5:HD:221:GLU:HG2 | 2.42 | 0.53 |
| 7:HI:349:TRP:N | 7:HI:520:ASN:O | 2.38 | 0.53 |
| 5:I:175:THR:O | 5:I:232:LEU:N | 2.35 | 0.53 |
| 8:IA:82:ARG:HH12 | 8:IA:138:GLY:HA2 | 1.73 | 0.53 |
| 9:IC:62:PHE:HE2 | 9:IC:129:SER:H | 1.56 | 0.53 |
| 10:ID:333:ALA:HA | 12:IF:188:LEU:HD23 | 1.89 | 0.53 |
| 5:J:118:LYS:HA | 5:J:142:ARG:NH2 | 2.22 | 0.53 |
| 5:J:86:VAL:HG13 | 5:J:87:ASN:N | 2.23 | 0.53 |
| 6:L:135:GLU:HA | 6:L:138:ALA:HB3 | 1.89 | 0.53 |
| 6:N:135:GLU:HA | 6:N:138:ALA:HB3 | 1.89 | 0.53 |
| 7:Q:255:SER:HB3 | 7:Q:263:VAL:HG13 | 1.89 | 0.53 |
| 9:T:62:PHE:HE2 | 9:T:129:SER:H | 1.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:554:ILE:HG21 | 1:X:577:PHE:CD1 | 2.43 | 0.53 |
| 1:X:642:PHE:CZ | 1:X:644:ASN:HB2 | 2.43 | 0.53 |
| 1:Y:297:VAL:HG11 | 1:Y:300:ILE:HG23 | 1.90 | 0.53 |
| 13:YA:26[D]:ARG:HA | 13:YA:55[D]:MET:O | 2.07 | 0.53 |
| 13:YA:31[D]:VAL:O | 13:YA:35[D]:HIS:HB2 | 2.08 | 0.53 |
| 13:YA:437[C]:ASN:HB3 | 13:YA:439[C]:TYR:CE1 | 2.43 | 0.53 |
| 13:YA:565[A]:TYR:CE2 | 13:YC:567[A]:ILE:HG23 | 2.43 | 0.53 |
| 13:YA:18[B]:ARG:NH1 | 13:YA:77[B]:VAL:HG23 | 2.23 | 0.53 |
| 13:YA:18[C]:ARG:NH1 | 13:YA:77[C]:VAL:HG23 | 2.23 | 0.53 |
| 13:YB:31[A]:VAL:O | 13:YB:35[A]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:31[B]:VAL:O | 13:YB:35[B]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:437[E]:ASN:HB3 | 13:YB:439[E]:TYR:CE1 | 2.43 | 0.53 |
| 13:YB:522[A]:VAL:HG23 | 13:YC:516[A]:GLY:O | 2.08 | 0.53 |
| 14:YD:17[B]:PHE:CD2 | 14:YD:28[B]:PHE:HB3 | 2.43 | 0.53 |
| 14:YD:17[E]:PHE:CD2 | 14:YD:28[E]:PHE:HB3 | 2.43 | 0.53 |
| 14:YD:43[F]:SER:OG | 14:YD:45[F]:TYR:N | 2.40 | 0.53 |
| 14:YE:17[C]:PHE:CD2 | 14:YE:28[C]:PHE:HB3 | 2.43 | 0.53 |
| 14:YE:332[C]:GLN:OE1 | 14:YF:101[C]:GLY:HA2 | 2.08 | 0.53 |
| 14:YE:50[B]:GLY:O | 14:YE:109[B]:LEU:N | 2.38 | 0.53 |
| 14:YF:123[B]:PRO:HA | 14:YF:161[B]:PRO:HA | 1.90 | 0.53 |
| 14:YF:17[B]:PHE:CD2 | 14:YF:28[B]:PHE:HB3 | 2.43 | 0.53 |
| 14:YF:43[D]:SER:OG | 14:YF:45[D]:TYR:N | 2.41 | 0.53 |
| 14:YF:16[E]:LEU:HA | 14:YF:69[E]:ILE:O | 2.08 | 0.53 |
| 2:Z:180:ILE:HA | 2:Z:219:TRP:HH2 | 1.73 | 0.53 |
| 2:Z:191:TYR:HE1 | 2:Z:235:LYS:HA | 1.73 | 0.53 |
| 2:Z:287:LEU:HD12 | 2:Z:289:PHE:H | 1.73 | 0.53 |
| 1:A:522:LYS:HB3 | 1:A:533:ASP:HA | 1.90 | 0.53 |
| 5:AC:78:THR:HA | 5:AC:108:THR:HB | 1.90 | 0.53 |
| 5:AD:102:TRP:CE3 | 5:AD:131:SER:HB2 | 2.42 | 0.53 |
| 5:AD:303:PRO:HB3 | 5:AD:385:TRP:CZ2 | 2.42 | 0.53 |
| 5:AD:330:HIS:ND1 | 5:AD:355:ASP:HB2 | 2.23 | 0.53 |
| 5:AD:86:VAL:HG13 | 5:AD:87:ASN:N | 2.23 | 0.53 |
| 5:AE:118:LYS:HA | 5:AE:142:ARG:NH2 | 2.23 | 0.53 |
| 6:AF:29:VAL:O | 6:AF:32:ARG:N | 2.36 | 0.53 |
| 7:AJ:239:ASN:OD1 | 7:AJ:253:ARG:NH2 | 2.40 | 0.53 |
| 7:AJ:349:TRP:N | 7:AJ:520:ASN:O | 2.38 | 0.53 |
| 1:B:236:PHE:CE2 | 1:B:270:ILE:HD11 | 2.44 | 0.53 |
| 7:BA:365:GLY:O | 7:BA:392:LEU:N | 2.25 | 0.53 |
| 7:AI:441:GLN:N | 7:BA:513:ARG:O | 2.34 | 0.53 |
| 8:BB:82:ARG:HH12 | 8:BB:138:GLY:HA2 | 1.73 | 0.53 |
| 1:BH:554:ILE:HG21 | 1:BH:577:PHE:CD1 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:19:GLU:N | 1:BI:19:GLU:OE1 | 2.41 | 0.53 |
| 2:BJ:205:TYR:HB2 | 2:BJ:206:GLN:OE1 | 2.09 | 0.53 |
| 2:BJ:549:PRO:HA | 2:BJ:555:ARG:NH2 | 2.23 | 0.53 |
| 1:BI:402:ALA:HB2 | 2:BJ:741:GLU:HA | 1.90 | 0.53 |
| 2:BJ:981:GLN:CG | 2:BJ:982:LEU:H | 2.19 | 0.53 |
| 2:C:127:PHE:O | 2:C:130:ASN:N | 2.41 | 0.53 |
| 2:C:180:ILE:HA | 2:C:219:TRP:HH2 | 1.73 | 0.53 |
| 2:C:406:LEU:HD11 | 2:C:413:TRP:HA | 1.89 | 0.53 |
| 2:C:403:ILE:CG2 | 2:C:417:PHE:HB3 | 2.38 | 0.53 |
| 2:C:450:PHE:CZ | 2:C:473:TYR:HE1 | 2.27 | 0.53 |
| 2:C:450:PHE:HZ | 2:C:473:TYR:HE1 | 1.56 | 0.53 |
| 2:C:947:VAL:O | 3:D:117:ALA:HB1 | 2.07 | 0.53 |
| 2:C:986:ARG:HH22 | 3:D:323:ASP:CB | 2.21 | 0.53 |
| 3:CB:150:LYS:HA | 3:CB:160:TRP:CE3 | 2.42 | 0.53 |
| 5:CF:177:PHE:O | 5:CF:230:ILE:HG13 | 2.08 | 0.53 |
| 5:CG:90:ASN:HA | 5:CH:98:VAL:HG22 | 1.91 | 0.53 |
| 5:CH:212:PHE:HZ | 5:CH:230:ILE:HB | 1.74 | 0.53 |
| 5:CH:289:LYS:HE2 | 5:CH:370:HIS:CE1 | 2.42 | 0.53 |
| 5:CH:419:ASP:HB3 | 5:CH:436:VAL:HB | 1.89 | 0.53 |
| 7:DC:341:ILE:HG13 | 7:DD:341:ILE:HD11 | 1.90 | 0.53 |
| 7:DC:440:GLN:OE1 | 7:DC:511:GLU:HG3 | 2.08 | 0.53 |
| 7:DD:372:CYS:SG | 7:DD:525:VAL:HB | 2.49 | 0.53 |
| 10:DH:205:LYS:HE2 | 10:DH:207:PHE:HE1 | 1.73 | 0.53 |
| 12:DJ:127:SER:HB3 | 12:DJ:161:SER:OG | 2.08 | 0.53 |
| 2:EC:101:GLU:OE1 | 2:EC:101:GLU:N | 2.41 | 0.53 |
| 2:EC:355:MET:HG3 | 2:EC:413:TRP:HE1 | 1.74 | 0.53 |
| 2:EC:986:ARG:HH22 | 3:ED:323:ASP:CB | 2.21 | 0.53 |
| 3:ED:150:LYS:HA | 3:ED:160:TRP:CE3 | 2.43 | 0.53 |
| 4:EH:201:LYS:HB3 | 4:EH:280:ALA:HB3 | 1.90 | 0.53 |
| 5:EI:67:SER:HB2 | 5:EI:94:ARG:HB2 | 1.91 | 0.53 |
| 5:EJ:102:TRP:CE3 | 5:EJ:131:SER:HB2 | 2.42 | 0.53 |
| 5:EJ:191:ILE:H | 5:FA:164:ARG:HH21 | 1.57 | 0.53 |
| 5:FA:20:ARG:HH12 | 5:FA:24:ILE:HD12 | 1.73 | 0.53 |
| 5:EJ:472:TYR:HA | 5:FA:416:ILE:HG23 | 1.90 | 0.53 |
| 7:FG:233:GLN:HE21 | 7:FG:237:ASN:HD21 | 1.56 | 0.53 |
| 7:FF:359:TRP:NE1 | 7:FG:340:THR:O | 2.35 | 0.53 |
| 8:DF:115:GLN:HG2 | 8:FI:79:HIS:HE2 | 1.74 | 0.53 |
| 10:GA:205:LYS:HE2 | 10:GA:207:PHE:HE1 | 1.73 | 0.53 |
| 12:GC:127:SER:HB3 | 12:GC:161:SER:OG | 2.08 | 0.53 |
| 1:GD:353:PHE:CD2 | 1:GD:392:ILE:HD13 | 2.44 | 0.53 |
| 1:GD:45:ASP:OD1 | 1:GD:46:TYR:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:986:ARG:HH22 | 3:GG:323:ASP:CB | 2.21 | 0.53 |
| 2:GF:790:THR:HA | 3:GH:82:LEU:HD13 | 1.89 | 0.53 |
| 4:GI:7:LYS:HB2 | 4:HA:39:TYR:CD1 | 2.43 | 0.53 |
| 4:GJ:131:LYS:N | 4:GJ:160:TRP:O | 2.29 | 0.53 |
| 5:HC:94:ARG:HD3 | 5:HC:134:GLU:HG2 | 1.89 | 0.53 |
| 5:HC:67:SER:HB2 | 5:HC:94:ARG:HB2 | 1.90 | 0.53 |
| 7:HH:118:PRO:HG3 | 7:HI:106:ALA:HA | 1.90 | 0.53 |
| 5:I:117:ILE:HG22 | 5:I:143:TRP:CE3 | 2.44 | 0.53 |
| 8:IA:23:VAL:HA | 8:IA:113:VAL:HA | 1.90 | 0.53 |
| 8:IA:17:ARG:NH2 | 8:IA:118:ARG:HD3 | 2.23 | 0.53 |
| 11:IE:54:PRO:HG2 | 11:IE:59:LEU:HB2 | 1.90 | 0.53 |
| 5:J:322:GLY:C | 5:J:359:GLU:HA | 2.28 | 0.53 |
| 5:K:186:TYR:HB3 | 5:K:227:GLY:O | 2.08 | 0.53 |
| 5:K:31:ASP:O | 5:K:35:TYR:N | 2.27 | 0.53 |
| 1:Y:19:GLU:OE1 | 1:Y:19:GLU:N | 2.41 | 0.53 |
| 13:YB:18[B]:ARG:NH1 | 13:YB:77[B]:VAL:HG23 | 2.23 | 0.53 |
| 13:YB:26[A]:ARG:HA | 13:YB:55[A]:MET:O | 2.07 | 0.53 |
| 13:YB:26[D]:ARG:HA | 13:YB:55[D]:MET:O | 2.07 | 0.53 |
| 13:YB:31[E]:VAL:O | 13:YB:35[E]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:425[B]:SER:HB2 | 13:YB:426[B]:PRO:HD2 | 1.89 | 0.53 |
| 13:YB:425[D]:SER:HB2 | 13:YB:426[D]:PRO:HD2 | 1.89 | 0.53 |
| 13:YB:437[F]:ASN:HB3 | 13:YB:439[F]:TYR:CE1 | 2.42 | 0.53 |
| 13:YB:529[D]:THR:N | 13:YC:520[D]:THR:O | 2.41 | 0.53 |
| 13:YC:31[B]:VAL:O | 13:YC:35[B]:HIS:HB2 | 2.08 | 0.53 |
| 13:YC:16[B]:GLU:OE2 | 13:YC:39[B]:ARG:NH2 | 2.42 | 0.53 |
| 13:YC:437[E]:ASN:HB3 | 13:YC:439[E]:TYR:CE1 | 2.43 | 0.53 |
| 13:YB:460[D]:GLY:N | 13:YC:452[D]:GLY:O | 2.41 | 0.53 |
| 13:YA:466[E]:ASN:HB2 | 13:YC:474[E]:ILE:HG12 | 1.89 | 0.53 |
| 13:YB:529[C]:THR:N | 13:YC:520[C]:THR:O | 2.41 | 0.53 |
| 14:YD:178[B]:LEU:HD11 | 14:YD:183[B]:ASP:HA | 1.89 | 0.53 |
| 14:YD:178[F]:LEU:HD11 | 14:YD:183[F]:ASP:HA | 1.89 | 0.53 |
| 14:YD:43[A]:SER:OG | 14:YD:45[A]:TYR:N | 2.41 | 0.53 |
| 14:YD:16[C]:LEU:HA | 14:YD:69[C]:ILE:O | 2.08 | 0.53 |
| 14:YE:17[A]:PHE:CD2 | 14:YE:28[A]:PHE:HB3 | 2.43 | 0.53 |
| 14:YF:16[B]:LEU:HA | 14:YF:69[B]:ILE:O | 2.08 | 0.53 |
| 2:Z:183:VAL:HA | 2:Z:210:LYS:HE3 | 1.90 | 0.53 |
| 1:A:45:ASP:OD1 | 1:A:46:TYR:N | 2.41 | 0.53 |
| 4:AB:161:ASN:OD1 | 4:AB:162:TYR:N | 2.41 | 0.53 |
| 5:AC:117:ILE:HG22 | 5:AC:143:TRP:CE3 | 2.44 | 0.53 |
| 5:AC:488:VAL:HG22 | 5:AE:486:VAL:HG12 | 1.90 | 0.53 |
| 5:AE:36:GLU:HA | 5:AE:50:LYS:HZ1 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AF:54:SER:O | 6:AG:164:GLN:NE2 | 2.41 | 0.53 |
| 6:AH:135:GLU:HA | 6:AH:138:ALA:HB3 | 1.89 | 0.53 |
| 7:AI:383:TYR:CD1 | 7:AI:393:PRO:HG3 | 2.44 | 0.53 |
| 1:B:297:VAL:HG11 | 1:B:300:ILE:HG23 | 1.90 | 0.53 |
| 1:B:510:MET:HB3 | 1:B:542:SER:HB3 | 1.89 | 0.53 |
| 9:BD:62:PHE:HE2 | 9:BD:129:SER:H | 1.56 | 0.53 |
| 12:BG:149:ARG:HB3 | 10:DH:212:THR:HG21 | 1.90 | 0.53 |
| 2:BJ:39:ALA:HB1 | 2:BJ:54:TYR:CE1 | 2.42 | 0.53 |
| 2:BJ:417:PHE:CZ | 2:BJ:423:GLU:HB3 | 2.44 | 0.53 |
| 2:BJ:450:PHE:CD1 | 2:BJ:453:ASP:HB2 | 2.43 | 0.53 |
| 2:C:148:ASN:HA | 2:C:168:ILE:HD13 | 1.90 | 0.53 |
| 2:C:193:MET:HG3 | 2:C:238:TYR:CE1 | 2.44 | 0.53 |
| 2:C:555:ARG:HD3 | 2:C:557:VAL:HB | 1.90 | 0.53 |
| 2:C:935:LYS:HZ2 | 2:C:936:LEU:HD13 | 1.72 | 0.53 |
| 4:CD:161:ASN:OD1 | 4:CD:162:TYR:N | 2.41 | 0.53 |
| 4:CE:111:ASN:HD21 | 4:CE:116:ILE:H | 1.56 | 0.53 |
| 5:CG:102:TRP:CE3 | 5:CG:131:SER:HB2 | 2.42 | 0.53 |
| 5:CG:94:ARG:HD3 | 5:CG:134:GLU:HG2 | 1.89 | 0.53 |
| 5:CG:358:VAL:HG22 | 5:CG:371:PHE:HB2 | 1.89 | 0.53 |
| 5:CH:357:SER:OG | 6:CJ:4:LEU:HD21 | 2.09 | 0.53 |
| 7:DC:349:TRP:N | 7:DC:520:ASN:O | 2.38 | 0.53 |
| 1:EB:236:PHE:CE2 | 1:EB:270:ILE:HD11 | 2.44 | 0.53 |
| 2:EC:127:PHE:O | 2:EC:130:ASN:N | 2.41 | 0.53 |
| 2:EC:193:MET:HG3 | 2:EC:238:TYR:CE1 | 2.44 | 0.53 |
| 2:EC:479:TRP:CD2 | 2:EC:505:PRO:HA | 2.43 | 0.53 |
| 2:EC:935:LYS:HZ2 | 2:EC:936:LEU:HD13 | 1.72 | 0.53 |
| 3:EE:133:CYS:HB2 | 3:EE:188:TRP:CZ3 | 2.43 | 0.53 |
| 4:EF:111:ASN:OD1 | 4:EF:114:GLY:N | 2.41 | 0.53 |
| 4:EG:131:LYS:HD2 | 4:EG:151:ILE:HD13 | 1.91 | 0.53 |
| 5:EI:177:PHE:O | 5:EI:230:ILE:HG13 | 2.08 | 0.53 |
| 5:FA:289:LYS:HE2 | 5:FA:370:HIS:CE1 | 2.42 | 0.53 |
| 5:FA:339:GLU:HG2 | 6:FB:173:THR:HB | 1.89 | 0.53 |
| 6:FD:135:GLU:HA | 6:FD:138:ALA:HB3 | 1.89 | 0.53 |
| 1:GD:554:ILE:HG21 | 1:GD:577:PHE:CD1 | 2.43 | 0.53 |
| 1:GE:544:ASP:OD1 | 1:GE:545:ARG:N | 2.41 | 0.53 |
| 1:GE:65:LEU:HD21 | 11:IE:70:TYR:OH | 2.08 | 0.53 |
| 2:GF:450:PHE:CZ | 2:GF:473:TYR:HE1 | 2.27 | 0.53 |
| 4:H:111:ASN:OD1 | 4:H:114:GLY:N | 2.41 | 0.53 |
| 5:HC:261:ARG:NE | 5:HC:297:GLY:O | 2.30 | 0.53 |
| 5:HC:396:LYS:O | 5:HC:399:ILE:HG13 | 2.08 | 0.53 |
| 5:HD:18:TYR:HB2 | 5:HD:21:LYS:H | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:3:GLN:HG3 | 5:HD:25:LYS:HG3 | 1.88 | 0.53 |
| 5:HD:419:ASP:HB3 | 5:HD:436:VAL:HB | 1.89 | 0.53 |
| 6:HF:135:GLU:HA | 6:HF:138:ALA:HB3 | 1.89 | 0.53 |
| 7:HI:36:ILE:HG13 | 7:HJ:18:PHE:HE1 | 1.73 | 0.53 |
| 7:HJ:211:SER:N | 7:HJ:214:THR:OG1 | 2.39 | 0.53 |
| 5:I:319:GLU:OE2 | 5:I:324:VAL:HG13 | 2.08 | 0.53 |
| 5:J:117:ILE:HG22 | 5:J:143:TRP:CE3 | 2.42 | 0.53 |
| 5:J:396:LYS:O | 5:J:399:ILE:HG13 | 2.08 | 0.53 |
| 5:K:172:GLN:HG2 | 5:K:173:GLY:H | 1.73 | 0.53 |
| 5:K:185:SER:HB2 | 5:K:228:PHE:HE1 | 1.72 | 0.53 |
| 5:K:212:PHE:HZ | 5:K:230:ILE:HB | 1.74 | 0.53 |
| 7:P:134:SER:HB3 | 7:P:140:GLY:N | 2.23 | 0.53 |
| 7:P:289:GLN:OE1 | 7:P:294:GLN:NE2 | 2.40 | 0.53 |
| 7:O:78:PRO:HB3 | 7:P:66:VAL:HA | 1.88 | 0.53 |
| 7:Q:233:GLN:HE21 | 7:Q:237:ASN:HD21 | 1.56 | 0.53 |
| 8:R:17:ARG:NH2 | 8:R:118:ARG:HD3 | 2.23 | 0.53 |
| 13:YA:31[C]:VAL:O | 13:YA:35[C]:HIS:HB2 | 2.08 | 0.53 |
| 13:YA:425[F]:SER:HB2 | 13:YA:426[F]:PRO:HD2 | 1.89 | 0.53 |
| 13:YA:461[A]:SER:OG | 13:YC:468[A]:ASP:OD2 | 2.26 | 0.53 |
| 13:YA:18[D]:ARG:NH1 | 13:YA:77[D]:VAL:HG23 | 2.23 | 0.53 |
| 13:YB:31[C]:VAL:O | 13:YB:35[C]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:527[A]:THR:O | 13:YC:519[A]:THR:HA | 2.08 | 0.53 |
| 13:YB:529[E]:THR:N | 13:YC:520[E]:THR:O | 2.41 | 0.53 |
| 13:YC:18[D]:ARG:NH1 | 13:YC:77[D]:VAL:HG23 | 2.23 | 0.53 |
| 13:YC:425[B]:SER:HB2 | 13:YC:426[B]:PRO:HD2 | 1.89 | 0.53 |
| 13:YA:466[D]:ASN:HB2 | 13:YC:474[D]:ILE:HG12 | 1.89 | 0.53 |
| 13:YB:522[B]:VAL:HG23 | 13:YC:516[B]:GLY:O | 2.08 | 0.53 |
| 13:YA:565[B]:TYR:CE2 | 13:YC:567[B]:ILE:HG23 | 2.44 | 0.53 |
| 13:YA:59[D]:GLN:CA | 13:YC:61[D]:ILE:HG21 | 2.30 | 0.53 |
| 14:YD:16[F]:LEU:HA | 14:YD:69[F]:ILE:O | 2.08 | 0.53 |
| 13:YA:90[D]:TRP:NE1 | 14:YD:175[D]:GLU:OE1 | 2.37 | 0.53 |
| 14:YD:17[D]:PHE:CD2 | 14:YD:28[D]:PHE:HB3 | 2.43 | 0.53 |
| 14:YD:43[C]:SER:OG | 14:YD:45[C]:TYR:N | 2.41 | 0.53 |
| 14:YE:123[A]:PRO:HA | 14:YE:161[A]:PRO:HA | 1.90 | 0.53 |
| 14:YE:123[B]:PRO:HA | 14:YE:161[B]:PRO:HA | 1.90 | 0.53 |
| 14:YE:238[D]:THR:OG1 | 14:YF:92[D]:HIS:NE2 | 2.42 | 0.53 |
| 14:YE:43[D]:SER:OG | 14:YE:45[D]:TYR:N | 2.41 | 0.53 |
| 14:YF:50[E]:GLY:O | 14:YF:109[E]:LEU:N | 2.37 | 0.53 |
| 2:Z:479:TRP:CD2 | 2:Z:505:PRO:HA | 2.43 | 0.53 |
| 2:Z:403:ILE:HD13 | 2:Z:501:PHE:HE2 | 1.72 | 0.53 |
| 2:Z:919:TYR:HA | 2:Z:990:MET:HE3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:981:GLN:CG | 2:Z:982:LEU:H | 2.19 | 0.53 |
| 15:ZA:2[F]:SER:N | 15:ZA:96[F]:ILE:O | 2.42 | 0.53 |
| 1:A:238:PHE:CE1 | 1:A:262:PRO:HD2 | 2.43 | 0.53 |
| 1:A:525:ASN:O | 1:A:528:THR:OG1 | 2.11 | 0.53 |
| 4:AA:161:ASN:OD1 | 4:AA:162:TYR:N | 2.41 | 0.53 |
| 4:AB:111:ASN:OD1 | 4:AB:114:GLY:N | 2.41 | 0.53 |
| 5:AC:391:GLY:O | 5:AC:392:THR:OG1 | 2.23 | 0.53 |
| 5:AD:137:TYR:HA | 5:AD:143:TRP:HD1 | 1.73 | 0.53 |
| 5:AD:322:GLY:C | 5:AD:359:GLU:HA | 2.28 | 0.53 |
| 5:AD:98:VAL:CG1 | 5:AD:99:PHE:HD2 | 2.21 | 0.53 |
| 5:AE:186:TYR:HB3 | 5:AE:227:GLY:O | 2.08 | 0.53 |
| 5:AE:36:GLU:HA | 5:AE:50:LYS:NZ | 2.24 | 0.53 |
| 5:AE:506:LEU:HB3 | 5:AE:510:GLY:HA2 | 1.89 | 0.53 |
| 5:I:77:VAL:HG23 | 7:AJ:167:GLN:NE2 | 232.13 | 0.53 |
| 7:AJ:228:ILE:O | 7:BA:225:LYS:HA | 2.09 | 0.53 |
| 7:BA:233:GLN:HE21 | 7:BA:237:ASN:HD21 | 1.56 | 0.53 |
| 10:BE:129:LEU:HD13 | 10:BE:209:TRP:HZ3 | 1.70 | 0.53 |
| 2:BJ:479:TRP:CD2 | 2:BJ:505:PRO:HA | 2.43 | 0.53 |
| 2:C:205:TYR:HB2 | 2:C:206:GLN:OE1 | 2.09 | 0.53 |
| 2:C:177:GLN:HG3 | 2:C:215:LYS:HB2 | 1.90 | 0.53 |
| 2:C:355:MET:HG3 | 2:C:413:TRP:HE1 | 1.74 | 0.53 |
| 2:C:479:TRP:CD2 | 2:C:505:PRO:HA | 2.44 | 0.53 |
| 2:C:91:GLN:NE2 | 2:C:92:SER:H | 2.06 | 0.53 |
| 3:CA:150:LYS:HA | 3:CA:160:TRP:CE3 | 2.43 | 0.53 |
| 2:BJ:790:THR:HA | 3:CB:82:LEU:HD13 | 1.90 | 0.53 |
| 5:CF:488:VAL:HG22 | 5:CH:486:VAL:HG12 | 1.90 | 0.53 |
| 5:CG:67:SER:HB2 | 5:CG:94:ARG:HB2 | 1.90 | 0.53 |
| 5:CG:98:VAL:CG1 | 5:CG:99:PHE:HD2 | 2.21 | 0.53 |
| 7:DC:36:ILE:HG13 | 7:DD:18:PHE:HE1 | 1.73 | 0.53 |
| 7:DD:354:LEU:HG | 7:DD:361:PHE:CZ | 2.42 | 0.53 |
| 8:DE:17:ARG:NH2 | 8:DE:118:ARG:HD3 | 2.23 | 0.53 |
| 8:DE:67:ASP:OD1 | 8:DE:68:ASP:N | 2.42 | 0.53 |
| 8:DF:82:ARG:HH12 | 8:DF:138:GLY:HA2 | 1.73 | 0.53 |
| 9:DG:62:PHE:HE2 | 9:DG:129:SER:H | 1.56 | 0.53 |
| 1:EA:485:VAL:HG22 | 1:EA:624:TYR:HD1 | 1.72 | 0.53 |
| 1:EB:19:GLU:OE1 | 1:EB:19:GLU:N | 2.41 | 0.53 |
| 4:EF:124:ILE:HD12 | 4:EF:137:LEU:HD23 | 1.90 | 0.53 |
| 5:EJ:67:SER:HB2 | 5:EJ:94:ARG:HB2 | 1.90 | 0.53 |
| 5:FA:31:ASP:O | 5:FA:35:TYR:N | 2.27 | 0.53 |
| 7:FE:130:GLU:HA | 7:FF:139:ASN:HD21 | 1.73 | 0.53 |
| 7:FE:29:ILE:O | 7:FE:30:THR:OG1 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:161:ASN:OD1 | 4:G:162:TYR:N | 2.41 | 0.53 |
| 4:G:201:LYS:HB3 | 4:G:280:ALA:HB3 | 1.90 | 0.53 |
| 1:GE:297:VAL:HG11 | 1:GE:300:ILE:HG23 | 1.90 | 0.53 |
| 1:GE:67:ILE:HA | 1:GE:70:PHE:HB3 | 1.90 | 0.53 |
| 2:GF:127:PHE:O | 2:GF:130:ASN:N | 2.41 | 0.53 |
| 2:GF:241:SER:O | 2:GF:244:THR:OG1 | 2.26 | 0.53 |
| 2:GF:369:ASP:OD1 | 2:GF:436:THR:HG23 | 2.08 | 0.53 |
| 2:GF:450:PHE:HZ | 2:GF:473:TYR:HE1 | 1.56 | 0.53 |
| 2:GF:768:TYR:CG | 3:GH:197:ASP:HB3 | 2.44 | 0.53 |
| 4:F:166:SER:H | 4:H:172:GLU:HA | 1.73 | 0.53 |
| 5:HB:177:PHE:O | 5:HB:230:ILE:HG13 | 2.08 | 0.53 |
| 5:HB:67:SER:HB2 | 5:HB:94:ARG:HB2 | 1.91 | 0.53 |
| 5:HD:289:LYS:O | 5:HD:290:SER:OG | 2.25 | 0.53 |
| 6:HG:100:PRO:O | 6:HG:103:SER:OG | 2.18 | 0.53 |
| 7:HH:110:VAL:HG12 | 7:HH:111:ASN:H | 1.74 | 0.53 |
| 7:HH:447:HIS:CD2 | 7:HJ:447:HIS:HD2 | 2.26 | 0.53 |
| 5:I:206:PHE:CG | 5:I:223:VAL:HA | 2.44 | 0.53 |
| 5:I:468:ASN:OD1 | 5:I:478:TRP:HB2 | 2.09 | 0.53 |
| 8:IB:23:VAL:HA | 8:IB:113:VAL:HA | 1.90 | 0.53 |
| 11:IE:31:ASN:OD1 | 11:IE:32:TYR:N | 2.41 | 0.53 |
| 5:J:318:GLN:HB3 | 6:L:4:LEU:HG | 1.91 | 0.53 |
| 5:J:67:SER:HB2 | 5:J:94:ARG:HB2 | 1.90 | 0.53 |
| 5:I:264:ARG:HB3 | 5:K:326:MET:HE1 | 1.89 | 0.53 |
| 7:O:90:ALA:HB2 | 7:O:96:GLY:N | 2.24 | 0.53 |
| 7:Q:173:ILE:O | 7:Q:178:PRO:HD2 | 2.09 | 0.53 |
| 10:U:132:SER:OG | 10:U:135:ASP:HB2 | 2.08 | 0.53 |
| 12:W:127:SER:HB3 | 12:W:161:SER:OG | 2.09 | 0.53 |
| 12:W:184:PRO:HA | 12:IF:153:ARG:HH12 | 1.71 | 0.53 |
| 1:X:87:SER:OG | 1:X:230:ILE:O | 2.21 | 0.53 |
| 13:YA:76[F]:PRO:HA | 13:YC:61[F]:ILE:HG22 | 1.89 | 0.53 |
| 13:YB:18[D]:ARG:HG3 | 13:YC:388[D]:PRO:HG3 | 1.91 | 0.53 |
| 13:YB:31[D]:VAL:O | 13:YB:35[D]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:527[B]:THR:O | 13:YC:519[B]:THR:HA | 2.09 | 0.53 |
| 13:YB:61[D]:ILE:HA | 13:YC:76[D]:PRO:C | 2.28 | 0.53 |
| 13:YC:18[B]:ARG:NH1 | 13:YC:77[B]:VAL:HG23 | 2.23 | 0.53 |
| 13:YC:26[A]:ARG:HA | 13:YC:55[A]:MET:O | 2.07 | 0.53 |
| 13:YC:31[F]:VAL:O | 13:YC:35[F]:HIS:HB2 | 2.08 | 0.53 |
| 13:YC:437[C]:ASN:HB3 | 13:YC:439[C]:TYR:CE1 | 2.43 | 0.53 |
| 13:YA:461[D]:SER:OG | 13:YC:468[D]:ASP:OD2 | 2.26 | 0.53 |
| 13:YA:519[E]:THR:HA | 13:YC:527[E]:THR:O | 2.07 | 0.53 |
| 13:YB:538[D]:VAL:HG11 | 13:YC:534[D]:LEU:CB | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:43[B]:SER:OG | 14:YD:45[B]:TYR:N | 2.41 | 0.53 |
| 14:YD:16[E]:LEU:HA | 14:YD:69[E]:ILE:O | 2.08 | 0.53 |
| 14:YE:123[D]:PRO:HA | 14:YE:161[D]:PRO:HA | 1.91 | 0.53 |
| 14:YE:16[A]:LEU:HA | 14:YE:69[A]:ILE:O | 2.08 | 0.53 |
| 10:GA:285:LEU:HA | 14:YE:215[C]:GLU:CG | 2.38 | 0.53 |
| 14:YE:43[C]:SER:OG | 14:YE:45[C]:TYR:N | 2.41 | 0.53 |
| 14:YE:50[A]:GLY:O | 14:YE:109[A]:LEU:N | 2.38 | 0.53 |
| 14:YE:73[D]:SER:OG | 14:YE:85[D]:THR:OG1 | 2.27 | 0.53 |
| 14:YE:73[E]:SER:OG | 14:YE:85[E]:THR:OG1 | 2.27 | 0.53 |
| 14:YF:17[A]:PHE:CD2 | 14:YF:28[A]:PHE:HB3 | 2.43 | 0.53 |
| 2:Z:193:MET:HG3 | 2:Z:238:TYR:CE1 | 2.44 | 0.53 |
| 2:Z:369:ASP:OD1 | 2:Z:436:THR:HG23 | 2.08 | 0.53 |
| 2:Z:355:MET:HG3 | 2:Z:413:TRP:HE1 | 1.74 | 0.53 |
| 2:Z:450:PHE:CZ | 2:Z:473:TYR:HE1 | 2.27 | 0.53 |
| 15:ZA:16[C]:ALA:HB3 | 15:ZA:48[C]:GLU:HB2 | 1.91 | 0.53 |
| 15:ZA:76[C]:GLN:HB3 | 15:ZA:96[C]:ILE:HD11 | 1.90 | 0.53 |
| 5:AE:166:GLU:OE1 | 5:AE:166:GLU:N | 2.42 | 0.53 |
| 7:AI:511:GLU:HB3 | 7:AI:513:ARG:NH1 | 2.23 | 0.53 |
| 7:AI:78:PRO:HB3 | 7:AJ:66:VAL:HA | 1.89 | 0.53 |
| 8:BC:17:ARG:NH2 | 8:BC:118:ARG:HD3 | 2.23 | 0.53 |
| 1:BH:238:PHE:CE1 | 1:BH:262:PRO:HD2 | 2.44 | 0.53 |
| 2:BJ:101:GLU:N | 2:BJ:101:GLU:OE1 | 2.41 | 0.53 |
| 2:BJ:926:PRO:HD2 | 2:BJ:985:GLU:O | 2.07 | 0.53 |
| 2:C:101:GLU:N | 2:C:101:GLU:OE1 | 2.41 | 0.53 |
| 2:C:544:VAL:HG12 | 2:C:546:GLU:HB3 | 1.90 | 0.53 |
| 4:CC:111:ASN:OD1 | 4:CC:114:GLY:N | 2.41 | 0.53 |
| 4:CD:131:LYS:HD2 | 4:CD:151:ILE:HD13 | 1.91 | 0.53 |
| 4:CE:131:LYS:HD2 | 4:CE:151:ILE:HD13 | 1.91 | 0.53 |
| 4:CE:154:ASP:HB2 | 4:CE:157:THR:HB | 1.88 | 0.53 |
| 4:CC:166:SER:H | 4:CE:172:GLU:HA | 1.73 | 0.53 |
| 5:CF:419:ASP:HB3 | 5:CF:436:VAL:HB | 1.88 | 0.53 |
| 5:CG:330:HIS:ND1 | 5:CG:355:ASP:HB2 | 2.23 | 0.53 |
| 7:DB:511:GLU:HB3 | 7:DB:513:ARG:NH1 | 2.23 | 0.53 |
| 7:DD:176:ILE:HG23 | 7:DD:177:ALA:H | 1.73 | 0.53 |
| 8:DE:14:ASP:OD2 | 8:DE:17:ARG:NH2 | 2.33 | 0.53 |
| 11:DI:36:PHE:HZ | 11:DI:76:CYS:HG | 1.55 | 0.53 |
| 1:BI:69:GLN:OE1 | 11:DI:70:TYR:HE1 | 1.91 | 0.53 |
| 12:DJ:247:VAL:HG12 | 12:DJ:248:MET:N | 2.23 | 0.53 |
| 1:EA:299:ASN:OD1 | 1:EA:300:ILE:N | 2.42 | 0.53 |
| 1:EA:642:PHE:CZ | 1:EA:644:ASN:HB2 | 2.43 | 0.53 |
| 1:EB:519:SER:HB3 | 1:EB:533:ASP:OD2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:191:TYR:HE1 | 2:EC:235:LYS:HA | 1.73 | 0.53 |
| 2:EC:935:LYS:HZ3 | 2:EC:936:LEU:HD13 | 1.71 | 0.53 |
| 2:EC:981:GLN:CG | 2:EC:982:LEU:H | 2.19 | 0.53 |
| 4:EF:131:LYS:HD2 | 4:EF:151:ILE:HD13 | 1.91 | 0.53 |
| 4:EF:161:ASN:OD1 | 4:EF:162:TYR:N | 2.41 | 0.53 |
| 5:EJ:426:ASP:O | 5:EJ:479:LYS:NZ | 2.42 | 0.53 |
| 5:FA:180:VAL:HG13 | 5:FA:181:PHE:H | 1.73 | 0.53 |
| 5:FA:196:ARG:HD2 | 7:FF:5:THR:OG1 | 2.08 | 0.53 |
| 5:FA:212:PHE:HZ | 5:FA:230:ILE:HB | 1.74 | 0.53 |
| 5:FA:36:GLU:HA | 5:FA:50:LYS:HZ1 | 1.74 | 0.53 |
| 5:EJ:90:ASN:HA | 5:FA:98:VAL:HG22 | 1.91 | 0.53 |
| 7:FE:140:GLY:HA2 | 7:FG:129:PHE:HZ | 1.72 | 0.53 |
| 7:FE:325:TYR:HD1 | 7:FE:330:ARG:HA | 1.72 | 0.53 |
| 7:FF:296:ILE:HG22 | 7:FF:298:GLY:H | 1.73 | 0.53 |
| 7:FF:210:ILE:O | 7:FG:210:ILE:HG22 | 2.09 | 0.53 |
| 8:FI:67:ASP:OD1 | 8:FI:68:ASP:N | 2.42 | 0.53 |
| 9:FJ:65:MET:SD | 9:FJ:97:PRO:HB2 | 2.48 | 0.53 |
| 12:GC:23:SER:N | 12:GC:202:ASN:O | 2.29 | 0.53 |
| 1:GE:510:MET:HB3 | 1:GE:542:SER:HB3 | 1.89 | 0.53 |
| 1:GE:83:ALA:O | 1:GE:326:ARG:NH2 | 2.36 | 0.53 |
| 2:GF:406:LEU:HD11 | 2:GF:413:TRP:HA | 1.89 | 0.53 |
| 2:GF:555:ARG:HD3 | 2:GF:557:VAL:HB | 1.90 | 0.53 |
| 2:EC:449:LYS:HD2 | 3:GG:74:HIS:NE2 | 2.24 | 0.53 |
| 3:GH:254:ASP:OD1 | 3:GH:255:SER:N | 2.41 | 0.53 |
| 5:HB:117:ILE:HG22 | 5:HB:143:TRP:CE3 | 2.44 | 0.53 |
| 5:HB:92:VAL:HG12 | 5:HB:136:VAL:HG12 | 1.91 | 0.53 |
| 5:HB:265:LEU:HG | 5:HB:379:ASP:HB2 | 1.90 | 0.53 |
| 5:HC:86:VAL:HG13 | 5:HC:87:ASN:N | 2.23 | 0.53 |
| 5:HD:127:ASN:HD21 | 5:HD:182:ARG:HH12 | 1.56 | 0.53 |
| 5:HD:316:ILE:HD13 | 6:HF:7:LYS:HG3 | 1.91 | 0.53 |
| 6:HG:135:GLU:HA | 6:HG:138:ALA:HB3 | 1.89 | 0.53 |
| 7:HH:29:ILE:O | 7:HH:30:THR:OG1 | 2.23 | 0.53 |
| 7:HH:322:THR:HG23 | 7:HI:327:GLN:HE21 | 1.73 | 0.53 |
| 7:HH:511:GLU:HB3 | 7:HH:513:ARG:NH1 | 2.23 | 0.53 |
| 7:HH:90:ALA:HB2 | 7:HH:96:GLY:N | 2.24 | 0.53 |
| 7:HH:100:TYR:OH | 7:HI:113:GLU:HG3 | 2.09 | 0.53 |
| 7:HI:325:TYR:CD1 | 7:HI:330:ARG:HA | 2.41 | 0.53 |
| 7:HI:93:THR:HG22 | 7:HI:94:VAL:HG23 | 1.89 | 0.53 |
| 5:I:103:ASN:OD1 | 5:I:104:VAL:N | 2.39 | 0.53 |
| 8:FH:120:ALA:HB3 | 8:IB:99:ILE:O | 2.09 | 0.53 |
| 5:J:13:ASP:OD1 | 5:J:14:GLY:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:275:SER:OG | 5:K:282:VAL:N | 2.40 | 0.53 |
| 7:P:296:ILE:HG22 | 7:P:298:GLY:H | 1.73 | 0.53 |
| 1:Y:544:ASP:OD1 | 1:Y:545:ARG:N | 2.41 | 0.53 |
| 13:YA:31[B]:VAL:O | 13:YA:35[B]:HIS:HB2 | 2.08 | 0.53 |
| 13:YA:31[E]:VAL:O | 13:YA:35[E]:HIS:HB2 | 2.08 | 0.53 |
| 13:YA:437[B]:ASN:HB3 | 13:YA:439[B]:TYR:CE1 | 2.43 | 0.53 |
| 13:YA:9[F]:ASN:HA | 13:YC:7[F]:ASN:ND2 | 2.17 | 0.53 |
| 13:YB:270[B]:ASN:O | 13:YB:274[B]:GLN:N | 2.42 | 0.53 |
| 13:YB:460[A]:GLY:N | 13:YC:452[A]:GLY:O | 2.41 | 0.53 |
| 13:YB:460[E]:GLY:N | 13:YC:452[E]:GLY:O | 2.42 | 0.53 |
| 13:YC:31[D]:VAL:O | 13:YC:35[D]:HIS:HB2 | 2.08 | 0.53 |
| 13:YC:31[A]:VAL:O | 13:YC:35[A]:HIS:HB2 | 2.08 | 0.53 |
| 13:YC:31[E]:VAL:O | 13:YC:35[E]:HIS:HB2 | 2.08 | 0.53 |
| 13:YB:71[E]:GLY:HA2 | 13:YC:393[E]:MET:HA | 1.91 | 0.53 |
| 13:YA:393[E]:MET:HA | 13:YC:71[E]:GLY:HA2 | 1.90 | 0.53 |
| 14:YD:123[D]:PRO:HA | 14:YD:161[D]:PRO:HA | 1.91 | 0.53 |
| 14:YD:16[D]:LEU:HA | 14:YD:69[D]:ILE:O | 2.08 | 0.53 |
| 14:YD:330[B]:LYS:HE3 | 14:YD:330[B]:LYS:HA | 1.91 | 0.53 |
| 14:YD:50[C]:GLY:O | 14:YD:109[C]:LEU:N | 2.38 | 0.53 |
| 14:YD:73[F]:SER:OG | 14:YD:85[F]:THR:OG1 | 2.27 | 0.53 |
| 14:YE:178[F]:LEU:HD11 | 14:YE:183[F]:ASP:HA | 1.89 | 0.53 |
| 14:YE:332[A]:GLN:OE1 | 14:YF:101[A]:GLY:HA2 | 2.09 | 0.53 |
| 2:Z:107:ALA:HB2 | 2:Z:128:THR:HA | 1.90 | 0.53 |
| 2:Z:450:PHE:CD1 | 2:Z:453:ASP:HB2 | 2.43 | 0.53 |
| 2:Z:549:PRO:HA | 2:Z:555:ARG:NH2 | 2.23 | 0.53 |
| 1:A:187:ILE:HD11 | 1:A:270:ILE:HD13 | 1.91 | 0.53 |
| 1:A:353:PHE:CD2 | 1:A:392:ILE:HD13 | 2.44 | 0.53 |
| 5:AC:92:VAL:HG12 | 5:AC:136:VAL:HG12 | 1.91 | 0.53 |
| 5:AE:79:ILE:HD11 | 5:AE:109:LEU:HG | 1.91 | 0.53 |
| 5:AE:127:ASN:HD21 | 5:AE:182:ARG:HH12 | 1.56 | 0.53 |
| 7:AJ:134:SER:HB3 | 7:AJ:140:GLY:N | 2.23 | 0.53 |
| 7:AJ:447:HIS:CD2 | 7:BA:447:HIS:CD2 | 2.97 | 0.53 |
| 8:BC:67:ASP:OD1 | 8:BC:68:ASP:N | 2.42 | 0.53 |
| 2:BJ:355:MET:HG3 | 2:BJ:413:TRP:HE1 | 1.74 | 0.53 |
| 2:BJ:91:GLN:NE2 | 2:BJ:92:SER:H | 2.06 | 0.53 |
| 2:C:417:PHE:CZ | 2:C:423:GLU:HB3 | 2.44 | 0.53 |
| 1:A:5:PRO:HG2 | 2:C:674:TYR:HA | 1.90 | 0.53 |
| 4:CD:53:GLY:O | 4:CE:7:LYS:HB3 | 2.09 | 0.53 |
| 5:CF:117:ILE:HG22 | 5:CF:143:TRP:CE3 | 2.44 | 0.53 |
| 5:CG:322:GLY:C | 5:CG:359:GLU:HA | 2.28 | 0.53 |
| 5:CG:426:ASP:O | 5:CG:479:LYS:NZ | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:85:THR:HB | 5:CG:137:TYR:CE2 | 2.44 | 0.53 |
| 5:CH:107:VAL:O | 5:CH:125:GLU:HG3 | 2.09 | 0.53 |
| 5:CH:166:GLU:OE1 | 5:CH:166:GLU:N | 2.42 | 0.53 |
| 6:DA:135:GLU:HA | 6:DA:138:ALA:HB3 | 1.89 | 0.53 |
| 7:DB:336:GLU:O | 7:DB:340:THR:N | 2.36 | 0.53 |
| 7:DD:457:LEU:HD23 | 7:DD:477:TRP:CZ2 | 2.43 | 0.53 |
| 8:DE:50:PRO:HB2 | 8:DE:57:LYS:HD3 | 1.91 | 0.53 |
| 8:DF:67:ASP:OD1 | 8:DF:68:ASP:N | 2.42 | 0.53 |
| 1:EA:353:PHE:CD2 | 1:EA:392:ILE:HD13 | 2.44 | 0.53 |
| 1:EA:554:ILE:HG21 | 1:EA:577:PHE:CD1 | 2.43 | 0.53 |
| 2:EC:543:LYS:HG2 | 2:EC:575:PHE:CZ | 2.43 | 0.53 |
| 3:EE:72:TRP:CD1 | 3:EE:304:ARG:HD3 | 2.44 | 0.53 |
| 4:EG:161:ASN:OD1 | 4:EG:162:TYR:N | 2.41 | 0.53 |
| 5:EJ:400:ILE:O | 5:EJ:403:THR:OG1 | 2.27 | 0.53 |
| 5:FA:6:ASN:OD1 | 5:FA:17:ASP:HB2 | 2.09 | 0.53 |
| 5:EJ:569:TYR:HE1 | 5:FA:544:VAL:HG22 | 1.74 | 0.53 |
| 7:FF:239:ASN:OD1 | 7:FF:253:ARG:NH2 | 2.40 | 0.53 |
| 8:FH:23:VAL:HA | 8:FH:113:VAL:HA | 1.90 | 0.53 |
| 8:FH:50:PRO:HB2 | 8:FH:57:LYS:HD3 | 1.91 | 0.53 |
| 8:FI:50:PRO:HB2 | 8:FI:57:LYS:HD3 | 1.91 | 0.53 |
| 10:GA:132:SER:OG | 10:GA:135:ASP:HB2 | 2.08 | 0.53 |
| 1:GE:19:GLU:N | 1:GE:19:GLU:OE1 | 2.41 | 0.53 |
| 1:GE:402:ALA:HB2 | 2:GF:741:GLU:HA | 1.91 | 0.53 |
| 1:GE:519:SER:HB3 | 1:GE:533:ASP:OD2 | 2.09 | 0.53 |
| 2:GF:355:MET:HG3 | 2:GF:413:TRP:HE1 | 1.74 | 0.53 |
| 2:GF:549:PRO:HA | 2:GF:555:ARG:NH2 | 2.23 | 0.53 |
| 5:HB:362:GLU:HB3 | 5:HB:367:GLU:OE1 | 2.08 | 0.53 |
| 5:HB:560:ASP:HB3 | 5:HB:561:GLU:OE1 | 2.09 | 0.53 |
| 5:HD:20:ARG:HH12 | 5:HD:24:ILE:HD12 | 1.73 | 0.53 |
| 5:HD:313:PHE:CD2 | 5:HD:320:LEU:HD21 | 2.44 | 0.53 |
| 5:HB:279:SER:HB2 | 5:HD:326:MET:HB2 | 1.90 | 0.53 |
| 5:HC:472:TYR:HA | 5:HD:416:ILE:HG23 | 1.89 | 0.53 |
| 7:HI:440:GLN:OE1 | 7:HI:511:GLU:HG3 | 2.08 | 0.53 |
| 7:HJ:34:ALA:HA | 7:HJ:37:ALA:HB3 | 1.91 | 0.53 |
| 7:HJ:372:CYS:SG | 7:HJ:525:VAL:HB | 2.49 | 0.53 |
| 5:I:201:TYR:HB3 | 5:J:166:GLU:HG2 | 1.90 | 0.53 |
| 5:I:177:PHE:O | 5:I:230:ILE:HG13 | 2.08 | 0.53 |
| 5:I:362:GLU:HB3 | 5:I:367:GLU:OE1 | 2.08 | 0.53 |
| 5:I:560:ASP:HB3 | 5:I:561:GLU:OE1 | 2.09 | 0.53 |
| 8:IB:36:CYS:HA | 8:IB:73:VAL:HG12 | 1.91 | 0.53 |
| 10:ID:286:VAL:HG22 | 10:ID:287:VAL:H | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:IF:127:SER:HB3 | 12:IF:161:SER:OG | 2.08 | 0.53 |
| 8:S:99:ILE:HD11 | 8:FI:55:ASN:HB3 | 1.91 | 0.53 |
| 1:X:238:PHE:CE1 | 1:X:262:PRO:HD2 | 2.44 | 0.53 |
| 1:Y:41:ASN:OD1 | 1:Y:42:GLU:N | 2.37 | 0.53 |
| 13:YA:148[F]:GLN:OE1 | 13:YA:381[F]:SER:HB2 | 2.09 | 0.53 |
| 13:YA:16[D]:GLU:OE2 | 13:YA:39[D]:ARG:NH2 | 2.41 | 0.53 |
| 13:YA:466[C]:ASN:HB2 | 13:YC:474[C]:ILE:HG12 | 1.89 | 0.53 |
| 13:YA:495[A]:THR:HA | 13:YC:503[A]:THR:O | 2.08 | 0.53 |
| 13:YB:425[E]:SER:HB2 | 13:YB:426[E]:PRO:HD2 | 1.89 | 0.53 |
| 13:YB:437[A]:ASN:HB3 | 13:YB:439[A]:TYR:CE1 | 2.43 | 0.53 |
| 13:YB:538[B]:VAL:HG11 | 13:YC:534[B]:LEU:CB | 2.38 | 0.53 |
| 13:YA:61[B]:ILE:HG23 | 13:YB:60[B]:PRO:HD3 | 1.90 | 0.53 |
| 13:YB:74[B]:THR:HG21 | 13:YC:388[B]:PRO:HB2 | 1.91 | 0.53 |
| 13:YB:18[E]:ARG:NH1 | 13:YB:77[E]:VAL:HG23 | 2.23 | 0.53 |
| 13:YC:437[D]:ASN:HB3 | 13:YC:439[D]:TYR:CE1 | 2.43 | 0.53 |
| 13:YB:474[C]:ILE:HD11 | 13:YC:470[C]:ARG:HD2 | 1.89 | 0.53 |
| 13:YA:495[D]:THR:HA | 13:YC:503[D]:THR:O | 2.08 | 0.53 |
| 13:YB:522[D]:VAL:HG23 | 13:YC:516[D]:GLY:O | 2.08 | 0.53 |
| 13:YA:60[B]:PRO:HD3 | 13:YC:61[B]:ILE:HG23 | 1.89 | 0.53 |
| 13:YA:90[B]:TRP:NE1 | 14:YD:175[B]:GLU:OE1 | 2.35 | 0.53 |
| 14:YE:232[D]:TYR:HD2 | 14:YE:233[D]:ASP:OD1 | 1.92 | 0.53 |
| 14:YF:123[E]:PRO:HA | 14:YF:161[E]:PRO:HA | 1.90 | 0.53 |
| 14:YF:43[B]:SER:OG | 14:YF:45[B]:TYR:N | 2.41 | 0.53 |
| 14:YF:43[C]:SER:OG | 14:YF:45[C]:TYR:N | 2.41 | 0.53 |
| 14:YF:73[C]:SER:OG | 14:YF:85[C]:THR:OG1 | 2.27 | 0.53 |
| 2:Z:91:GLN:NE2 | 2:Z:92:SER:H | 2.06 | 0.53 |
| 2:Z:969:TYR:O | 2:Z:973:ASN:N | 2.29 | 0.53 |
| 1:A:286:PHE:HB2 | 1:A:300:ILE:CD1 | 2.39 | 0.53 |
| 4:AA:39:TYR:CD1 | 4:AB:7:LYS:HB2 | 2.44 | 0.53 |
| 5:AC:289:LYS:HE2 | 5:AC:370:HIS:HE1 | 1.74 | 0.53 |
| 5:AD:90:ASN:HA | 5:AE:98:VAL:HG22 | 1.91 | 0.53 |
| 5:AE:6:ASN:OD1 | 5:AE:17:ASP:HB2 | 2.09 | 0.53 |
| 6:AG:17:PHE:O | 6:AH:13:ARG:NH1 | 2.28 | 0.53 |
| 5:AC:318:GLN:NE2 | 6:AH:4:LEU:HA | 2.24 | 0.53 |
| 7:AI:90:ALA:HB2 | 7:AI:96:GLY:N | 2.24 | 0.53 |
| 1:B:582:ASN:HD21 | 1:B:586:ARG:NH2 | 1.98 | 0.53 |
| 7:BA:255:SER:HB3 | 7:BA:263:VAL:HG13 | 1.89 | 0.53 |
| 1:BH:231:ASP:OD1 | 1:BH:233:ASN:N | 2.36 | 0.53 |
| 1:BH:187:ILE:HD11 | 1:BH:270:ILE:HD13 | 1.91 | 0.53 |
| 1:BI:236:PHE:CE2 | 1:BI:270:ILE:HD11 | 2.44 | 0.53 |
| 2:BJ:180:ILE:HA | 2:BJ:219:TRP:HH2 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:228:ARG:HD2 | 5:CH:556:GLN:HE22 | 1.74 | 0.53 |
| 2:BJ:207:PRO:HA | 2:BJ:229:VAL:HG23 | 1.91 | 0.53 |
| 2:BJ:7:SER:O | 2:BJ:28:VAL:HG11 | 2.09 | 0.53 |
| 2:BJ:544:VAL:HG12 | 2:BJ:546:GLU:HB3 | 1.90 | 0.53 |
| 2:BJ:548:ILE:HB | 2:BJ:555:ARG:HB3 | 1.89 | 0.53 |
| 2:C:287:LEU:HD12 | 2:C:289:PHE:H | 1.73 | 0.53 |
| 3:CB:133:CYS:HB2 | 3:CB:188:TRP:CZ3 | 2.44 | 0.53 |
| 3:CB:72:TRP:CD1 | 3:CB:304:ARG:HD3 | 2.44 | 0.53 |
| 5:CF:319:GLU:OE2 | 5:CF:324:VAL:HG13 | 2.08 | 0.53 |
| 5:CF:265:LEU:HG | 5:CF:379:ASP:HB2 | 1.90 | 0.53 |
| 5:CG:396:LYS:O | 5:CG:399:ILE:HG13 | 2.08 | 0.53 |
| 5:CG:44:TYR:CD2 | 5:CG:48:ALA:HB2 | 2.37 | 0.53 |
| 5:CG:86:VAL:HG13 | 5:CG:87:ASN:N | 2.23 | 0.53 |
| 5:CH:36:GLU:HA | 5:CH:50:LYS:NZ | 2.24 | 0.53 |
| 5:CG:569:TYR:OH | 5:CH:571:GLU:OE2 | 2.13 | 0.53 |
| 6:DA:195:LEU:HD13 | 6:DA:215:PHE:HE1 | 1.74 | 0.53 |
| 7:DB:512:THR:O | 7:DD:514:PRO:HB3 | 2.09 | 0.53 |
| 7:DC:134:SER:HB3 | 7:DC:140:GLY:N | 2.23 | 0.53 |
| 7:DC:296:ILE:HG22 | 7:DC:298:GLY:H | 1.73 | 0.53 |
| 2:EC:450:PHE:CZ | 2:EC:473:TYR:HE1 | 2.27 | 0.53 |
| 2:EC:544:VAL:HG12 | 2:EC:546:GLU:HB3 | 1.90 | 0.53 |
| 2:EC:555:ARG:HD3 | 2:EC:557:VAL:HB | 1.90 | 0.53 |
| 2:EC:900:ILE:HG13 | 3:EE:311:TYR:CE1 | 2.43 | 0.53 |
| 7:Q:495:GLN:NE2 | 5:EI:423:THR:O | 2.28 | 0.53 |
| 5:EI:94:ARG:CD | 5:EI:134:GLU:HG2 | 2.38 | 0.53 |
| 7:FE:146:SER:O | 7:FE:150:ALA:N | 2.38 | 0.53 |
| 7:FE:265:LEU:O | 7:FF:257:THR:HA | 2.08 | 0.53 |
| 7:FE:511:GLU:HB3 | 7:FE:513:ARG:NH1 | 2.23 | 0.53 |
| 7:FE:213:TYR:HB2 | 7:FF:203:THR:O | 2.08 | 0.53 |
| 7:FG:211:SER:N | 7:FG:214:THR:OG1 | 2.39 | 0.53 |
| 7:FG:457:LEU:HD23 | 7:FG:477:TRP:CZ2 | 2.43 | 0.53 |
| 8:FI:23:VAL:HA | 8:FI:113:VAL:HA | 1.90 | 0.53 |
| 8:DF:9:ALA:HB2 | 8:FI:34:PHE:HD2 | 1.73 | 0.53 |
| 4:G:111:ASN:OD1 | 4:G:114:GLY:N | 2.41 | 0.53 |
| 12:GC:126:TYR:CD2 | 12:GC:163:ARG:HG3 | 2.44 | 0.53 |
| 1:GD:447:TYR:HB2 | 1:GD:467:TYR:HD2 | 1.73 | 0.53 |
| 1:GD:80:MET:HG3 | 1:GD:81:ARG:HG3 | 1.90 | 0.53 |
| 4:GI:218:GLU:OE1 | 4:GJ:201:LYS:NZ | 2.31 | 0.53 |
| 4:GJ:161:ASN:OD1 | 4:GJ:162:TYR:N | 2.41 | 0.53 |
| 4:G:53:GLY:O | 4:H:7:LYS:HB3 | 2.09 | 0.53 |
| 5:HB:552:VAL:HG11 | 5:HD:569:TYR:CE2 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:400:ILE:O | 5:HC:403:THR:OG1 | 2.27 | 0.53 |
| 5:HC:501:LEU:HB3 | 5:HC:512:PRO:HB2 | 1.91 | 0.53 |
| 5:HD:186:TYR:HB3 | 5:HD:227:GLY:O | 2.08 | 0.53 |
| 5:HD:261:ARG:O | 5:HD:383:ILE:N | 2.38 | 0.53 |
| 5:HD:36:GLU:HA | 5:HD:50:LYS:NZ | 2.24 | 0.53 |
| 7:HH:161:THR:OG1 | 7:HH:164:LYS:HE3 | 2.09 | 0.53 |
| 7:HI:518:SER:HB3 | 7:HJ:403:SER:HA | 1.90 | 0.53 |
| 7:HJ:457:LEU:HD23 | 7:HJ:477:TRP:CZ2 | 2.43 | 0.53 |
| 8:IA:67:ASP:OD1 | 8:IA:68:ASP:N | 2.42 | 0.53 |
| 8:IB:82:ARG:HH12 | 8:IB:138:GLY:HA2 | 1.73 | 0.53 |
| 5:J:132:ASP:HB2 | 5:J:149:LYS:HG3 | 1.91 | 0.53 |
| 5:J:400:ILE:O | 5:J:403:THR:OG1 | 2.27 | 0.53 |
| 5:K:313:PHE:CD2 | 5:K:320:LEU:HD21 | 2.44 | 0.53 |
| 7:O:110:VAL:HG12 | 7:O:111:ASN:H | 1.74 | 0.53 |
| 7:P:228:ILE:O | 7:Q:225:LYS:HA | 2.09 | 0.53 |
| 13:YA:193[C]:ASP:OD1 | 13:YA:197[C]:TYR:N | 2.31 | 0.53 |
| 13:YA:461[F]:SER:OG | 13:YC:468[F]:ASP:OD2 | 2.27 | 0.53 |
| 13:YB:148[D]:GLN:OE1 | 13:YB:381[D]:SER:HB2 | 2.09 | 0.53 |
| 13:YB:148[F]:GLN:OE1 | 13:YB:381[F]:SER:HB2 | 2.09 | 0.53 |
| 13:YA:454[E]:LYS:NZ | 13:YB:464[E]:TYR:OH | 2.42 | 0.53 |
| 13:YB:554[F]:MET:HG3 | 13:YC:550[F]:TRP:HB2 | 1.91 | 0.53 |
| 13:YB:474[D]:ILE:HD11 | 13:YC:470[D]:ARG:HD2 | 1.89 | 0.53 |
| 13:YB:522[C]:VAL:HG23 | 13:YC:516[C]:GLY:O | 2.08 | 0.53 |
| 13:YA:520[F]:THR:O | 13:YC:529[F]:THR:N | 2.42 | 0.53 |
| 14:YD:232[E]:TYR:HD2 | 14:YD:233[E]:ASP:OD1 | 1.92 | 0.53 |
| 14:YF:17[F]:PHE:CD2 | 14:YF:28[F]:PHE:HB3 | 2.43 | 0.53 |
| 14:YF:73[D]:SER:OG | 14:YF:85[D]:THR:OG1 | 2.27 | 0.53 |
| 2:Z:206:GLN:C | 2:Z:208:VAL:H | 2.12 | 0.53 |
| 2:Z:207:PRO:HA | 2:Z:229:VAL:HG23 | 1.91 | 0.53 |
| 2:Z:417:PHE:CZ | 2:Z:423:GLU:HB3 | 2.44 | 0.53 |
| 1:A:345:TYR:OH | 1:A:400:ASN:OD1 | 2.25 | 0.53 |
| 5:AC:177:PHE:O | 5:AC:230:ILE:HG13 | 2.08 | 0.53 |
| 5:AC:265:LEU:HG | 5:AC:379:ASP:HB2 | 1.90 | 0.53 |
| 5:AC:94:ARG:CD | 5:AC:134:GLU:HG2 | 2.38 | 0.53 |
| 5:AC:201:TYR:HB3 | 5:AD:166:GLU:HG2 | 1.90 | 0.53 |
| 5:AD:400:ILE:O | 5:AD:403:THR:OG1 | 2.27 | 0.53 |
| 5:AE:107:VAL:O | 5:AE:125:GLU:HG3 | 2.09 | 0.53 |
| 5:AE:172:GLN:HG2 | 5:AE:173:GLY:H | 1.73 | 0.53 |
| 5:AE:212:PHE:HZ | 5:AE:230:ILE:HB | 1.74 | 0.53 |
| 5:AE:275:SER:OG | 5:AE:282:VAL:N | 2.40 | 0.53 |
| 7:AI:73:THR:HG23 | 7:AI:74:LYS:H | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:32:VAL:O | 7:AJ:36:ILE:HG12 | 2.08 | 0.53 |
| 1:B:19:GLU:N | 1:B:19:GLU:OE1 | 2.41 | 0.53 |
| 7:BA:34:ALA:HA | 7:BA:37:ALA:HB3 | 1.91 | 0.53 |
| 5:K:353:HIS:NE2 | 7:BA:476:ASP:HB2 | 2.23 | 0.53 |
| 9:BD:87:ARG:O | 9:BD:113:ILE:HG12 | 2.09 | 0.53 |
| 12:BG:127:SER:HB3 | 12:BG:161:SER:OG | 2.08 | 0.53 |
| 12:BG:247:VAL:HG12 | 12:BG:248:MET:N | 2.23 | 0.53 |
| 1:BH:508:ARG:NH2 | 1:BH:576:ASP:O | 2.42 | 0.53 |
| 2:BJ:193:MET:HG3 | 2:BJ:238:TYR:CE1 | 2.44 | 0.53 |
| 2:C:206:GLN:HG3 | 5:K:555:CYS:O | 2.09 | 0.53 |
| 2:C:183:VAL:HA | 2:C:210:LYS:HE3 | 1.90 | 0.53 |
| 4:CC:161:ASN:OD1 | 4:CC:162:TYR:N | 2.41 | 0.53 |
| 5:CG:180:VAL:HG13 | 5:CG:181:PHE:H | 1.72 | 0.53 |
| 5:CH:359:GLU:O | 5:CH:370:HIS:N | 2.36 | 0.53 |
| 7:DB:383:TYR:CD1 | 7:DB:393:PRO:HG3 | 2.44 | 0.53 |
| 7:DB:66:VAL:HG21 | 7:DB:80:THR:HB | 1.91 | 0.53 |
| 7:DC:228:ILE:O | 7:DD:225:LYS:HA | 2.09 | 0.53 |
| 5:CG:196:ARG:NE | 7:DD:5:THR:HG23 | 2.23 | 0.53 |
| 8:DF:50:PRO:HB2 | 8:DF:57:LYS:HD3 | 1.91 | 0.53 |
| 3:E:133:CYS:HB2 | 3:E:188:TRP:CZ3 | 2.43 | 0.53 |
| 2:C:816:LEU:HB2 | 3:E:201:ASN:HD22 | 1.74 | 0.53 |
| 2:EC:406:LEU:HD11 | 2:EC:413:TRP:HA | 1.89 | 0.53 |
| 2:EC:408:HIS:ND1 | 2:EC:410:GLU:OE2 | 2.42 | 0.53 |
| 2:EC:4:LYS:HA | 2:EC:90:GLU:HB3 | 1.91 | 0.53 |
| 2:EC:816:LEU:HB2 | 3:EE:201:ASN:HD22 | 1.73 | 0.53 |
| 4:EF:218:GLU:OE1 | 4:EG:201:LYS:NZ | 2.29 | 0.53 |
| 4:EH:161:ASN:OD1 | 4:EH:162:TYR:N | 2.41 | 0.53 |
| 5:EI:117:ILE:HG13 | 5:EI:118:LYS:H | 1.73 | 0.53 |
| 5:EI:117:ILE:HG22 | 5:EI:143:TRP:CE3 | 2.44 | 0.53 |
| 5:EI:255:ARG:NE | 5:FA:390:LEU:HD12 | 2.24 | 0.53 |
| 5:EJ:85:THR:HB | 5:EJ:137:TYR:CE2 | 2.44 | 0.53 |
| 4:F:111:ASN:OD1 | 4:F:114:GLY:N | 2.41 | 0.53 |
| 5:FA:118:LYS:HA | 5:FA:142:ARG:NH2 | 2.23 | 0.53 |
| 5:FA:172:GLN:HG2 | 5:FA:173:GLY:H | 1.73 | 0.53 |
| 6:FB:135:GLU:HA | 6:FB:138:ALA:HB3 | 1.89 | 0.53 |
| 6:FB:195:LEU:HD13 | 6:FB:215:PHE:HE1 | 1.74 | 0.53 |
| 7:FF:110:VAL:HG12 | 7:FF:111:ASN:H | 1.74 | 0.53 |
| 7:FF:289:GLN:OE1 | 7:FF:294:GLN:NE2 | 2.40 | 0.53 |
| 7:FF:440:GLN:OE1 | 7:FF:511:GLU:HG3 | 2.08 | 0.53 |
| 7:FF:341:ILE:HG13 | 7:FG:341:ILE:HD11 | 1.90 | 0.53 |
| 8:FI:36:CYS:HA | 8:FI:73:VAL:HG12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:GC:247:VAL:HG12 | 12:GC:248:MET:N | 2.23 | 0.53 |
| 1:GD:187:ILE:HD11 | 1:GD:270:ILE:HD13 | 1.91 | 0.53 |
| 1:GD:642:PHE:CZ | 1:GD:644:ASN:HB2 | 2.44 | 0.53 |
| 1:GE:236:PHE:CE2 | 1:GE:270:ILE:HD11 | 2.44 | 0.53 |
| 2:GF:207:PRO:HA | 2:GF:229:VAL:HG23 | 1.90 | 0.53 |
| 2:GF:351:GLU:CB | 2:GF:353:ASP:HB2 | 2.31 | 0.53 |
| 2:GF:326:VAL:HG11 | 2:GF:413:TRP:CZ2 | 2.44 | 0.53 |
| 3:GH:133:CYS:HB2 | 3:GH:188:TRP:CZ3 | 2.43 | 0.53 |
| 3:GH:72:TRP:CD1 | 3:GH:304:ARG:HD3 | 2.44 | 0.53 |
| 5:HB:117:ILE:HG13 | 5:HB:118:LYS:H | 1.73 | 0.53 |
| 5:HB:206:PHE:CG | 5:HB:223:VAL:HA | 2.44 | 0.53 |
| 5:HC:180:VAL:HG13 | 5:HC:181:PHE:H | 1.73 | 0.53 |
| 5:HC:317:LEU:HD13 | 5:HD:312:ARG:NH2 | 2.24 | 0.53 |
| 5:HD:180:VAL:HG13 | 5:HD:181:PHE:H | 1.73 | 0.53 |
| 5:HB:196:ARG:HG2 | 5:HD:198:ASN:O | 2.08 | 0.53 |
| 7:HI:47:VAL:HG12 | 7:HI:48:PRO:N | 2.24 | 0.53 |
| 8:IB:17:ARG:NH2 | 8:IB:118:ARG:HD3 | 2.23 | 0.53 |
| 9:IC:65:MET:SD | 9:IC:97:PRO:HB2 | 2.48 | 0.53 |
| 5:K:36:GLU:HA | 5:K:50:LYS:NZ | 2.24 | 0.53 |
| 7:O:49:ASP:O | 7:O:56:GLY:HA3 | 2.09 | 0.53 |
| 7:O:73:THR:HG23 | 7:O:74:LYS:H | 1.73 | 0.53 |
| 7:P:32:VAL:O | 7:P:36:ILE:HG12 | 2.08 | 0.53 |
| 7:P:359:TRP:NE1 | 7:Q:340:THR:O | 2.36 | 0.53 |
| 8:S:82:ARG:HH12 | 8:S:138:GLY:HA2 | 1.73 | 0.53 |
| 9:T:65:MET:SD | 9:T:97:PRO:HB2 | 2.48 | 0.53 |
| 11:V:54:PRO:HG2 | 11:V:59:LEU:HB2 | 1.90 | 0.53 |
| 1:X:353:PHE:CD2 | 1:X:392:ILE:HD13 | 2.44 | 0.53 |
| 1:Y:67:ILE:HA | 1:Y:70:PHE:HB3 | 1.90 | 0.53 |
| 13:YA:16[E]:GLU:OE2 | 13:YA:39[E]:ARG:NH2 | 2.42 | 0.53 |
| 13:YA:16[F]:GLU:OE2 | 13:YA:39[F]:ARG:NH2 | 2.42 | 0.53 |
| 13:YA:148[C]:GLN:OE1 | 13:YA:381[C]:SER:HB2 | 2.09 | 0.53 |
| 13:YA:520[A]:THR:O | 13:YC:529[A]:THR:N | 2.42 | 0.53 |
| 13:YB:270[E]:ASN:O | 13:YB:274[E]:GLN:N | 2.42 | 0.53 |
| 13:YB:270[F]:ASN:O | 13:YB:274[F]:GLN:N | 2.42 | 0.53 |
| 13:YB:527[C]:THR:O | 13:YC:519[C]:THR:HA | 2.08 | 0.53 |
| 13:YB:18[F]:ARG:NH1 | 13:YB:77[F]:VAL:HG23 | 2.23 | 0.53 |
| 13:YC:425[C]:SER:HB2 | 13:YC:426[C]:PRO:HD2 | 1.89 | 0.53 |
| 13:YB:61[B]:ILE:HG12 | 13:YC:60[B]:PRO:HD2 | 1.90 | 0.53 |
| 13:YC:18[F]:ARG:NH1 | 13:YC:77[F]:VAL:HG23 | 2.23 | 0.53 |
| 14:YD:123[C]:PRO:HA | 14:YD:161[C]:PRO:HA | 1.91 | 0.53 |
| 14:YE:123[F]:PRO:HA | 14:YE:161[F]:PRO:HA | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:17[B]:PHE:CD2 | 14:YE:28[B]:PHE:HB3 | 2.43 | 0.53 |
| 14:YE:16[C]:LEU:HA | 14:YE:69[C]:ILE:O | 2.08 | 0.53 |
| 2:Z:7:SER:O | 2:Z:28:VAL:HG11 | 2.09 | 0.53 |
| 2:Z:4:LYS:HA | 2:Z:90:GLU:HB3 | 1.91 | 0.53 |
| 1:A:80:MET:HG3 | 1:A:81:ARG:HG3 | 1.90 | 0.53 |
| 5:AE:196:ARG:NE | 7:AJ:5:THR:HG23 | 2.24 | 0.53 |
| 9:BD:65:MET:SD | 9:BD:97:PRO:HB2 | 2.48 | 0.53 |
| 10:BE:205:LYS:HB2 | 10:BE:311:PHE:HZ | 1.74 | 0.53 |
| 1:BH:336:GLN:HG2 | 1:BI:336:GLN:HG2 | 1.91 | 0.53 |
| 1:BH:522:LYS:HB3 | 1:BH:533:ASP:HA | 1.90 | 0.53 |
| 2:BJ:127:PHE:O | 2:BJ:130:ASN:N | 2.41 | 0.53 |
| 2:BJ:183:VAL:HA | 2:BJ:210:LYS:HE3 | 1.90 | 0.53 |
| 2:BJ:408:HIS:ND1 | 2:BJ:410:GLU:OE2 | 2.42 | 0.53 |
| 2:BJ:403:ILE:HD13 | 2:BJ:501:PHE:HE2 | 1.72 | 0.53 |
| 2:C:369:ASP:OD1 | 2:C:436:THR:HG23 | 2.08 | 0.53 |
| 2:C:4:LYS:HA | 2:C:90:GLU:HB3 | 1.91 | 0.53 |
| 2:C:549:PRO:HA | 2:C:555:ARG:NH2 | 2.23 | 0.53 |
| 4:CE:79:VAL:N | 4:CE:97:ILE:O | 2.31 | 0.53 |
| 5:CF:67:SER:HB2 | 5:CF:94:ARG:HB2 | 1.91 | 0.53 |
| 5:CG:132:ASP:HB2 | 5:CG:149:LYS:HG3 | 1.91 | 0.53 |
| 6:CI:195:LEU:HD13 | 6:CI:215:PHE:HE1 | 1.74 | 0.53 |
| 7:DB:161:THR:OG1 | 7:DB:164:LYS:HE3 | 2.09 | 0.53 |
| 7:DC:447:HIS:CD2 | 7:DD:447:HIS:CD2 | 2.96 | 0.53 |
| 12:DJ:125:ILE:HA | 12:DJ:162:PHE:CB | 2.39 | 0.53 |
| 3:E:72:TRP:CD1 | 3:E:304:ARG:HD3 | 2.44 | 0.53 |
| 2:EC:417:PHE:CZ | 2:EC:423:GLU:HB3 | 2.44 | 0.53 |
| 2:EC:549:PRO:HA | 2:EC:555:ARG:NH2 | 2.23 | 0.53 |
| 2:BJ:509:TYR:HB2 | 3:EE:175:ASP:OD2 | 2.09 | 0.53 |
| 4:EH:131:LYS:HD2 | 4:EH:151:ILE:HD13 | 1.91 | 0.53 |
| 5:EI:469:PRO:HB2 | 5:EI:478:TRP:CD1 | 2.44 | 0.53 |
| 5:EI:72:THR:HG22 | 5:EI:77:VAL:HG22 | 1.91 | 0.53 |
| 5:EJ:501:LEU:HB3 | 5:EJ:512:PRO:HB2 | 1.91 | 0.53 |
| 5:EJ:98:VAL:CG1 | 5:EJ:99:PHE:HD2 | 2.21 | 0.53 |
| 4:F:124:ILE:HD12 | 4:F:137:LEU:HD23 | 1.90 | 0.53 |
| 5:FA:206:PHE:CD2 | 5:FA:223:VAL:HA | 2.44 | 0.53 |
| 5:FA:36:GLU:HA | 5:FA:50:LYS:NZ | 2.24 | 0.53 |
| 6:FB:13:ARG:HB2 | 6:FD:10:VAL:HA | 1.89 | 0.53 |
| 7:FE:301:ARG:HB3 | 7:FG:295:ILE:HG13 | 1.90 | 0.53 |
| 7:FE:439:ILE:HG23 | 7:FG:515:TRP:CH2 | 2.43 | 0.53 |
| 10:GA:205:LYS:HB2 | 10:GA:311:PHE:HZ | 1.74 | 0.53 |
| 2:GF:205:TYR:HB2 | 2:GF:206:GLN:OE1 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:GJ:111:ASN:OD1 | 4:GJ:114:GLY:N | 2.41 | 0.53 |
| 4:GJ:27:GLY:HA2 | 4:GJ:30:LYS:HD2 | 1.91 | 0.53 |
| 4:HA:161:ASN:OD1 | 4:HA:162:TYR:N | 2.41 | 0.53 |
| 5:HB:94:ARG:CD | 5:HB:134:GLU:HG2 | 2.38 | 0.53 |
| 5:HD:323:THR:HG21 | 5:HD:354:THR:HG23 | 1.91 | 0.53 |
| 7:HI:228:ILE:O | 7:HJ:225:LYS:HA | 2.09 | 0.53 |
| 5:I:92:VAL:HG12 | 5:I:136:VAL:HG12 | 1.91 | 0.53 |
| 10:ID:205:LYS:HB2 | 10:ID:311:PHE:HZ | 1.74 | 0.53 |
| 12:IF:126:TYR:CD2 | 12:IF:163:ARG:HG3 | 2.44 | 0.53 |
| 5:J:137:TYR:HA | 5:J:143:TRP:HD1 | 1.72 | 0.53 |
| 5:J:426:ASP:O | 5:J:479:LYS:NZ | 2.42 | 0.53 |
| 5:K:180:VAL:HG13 | 5:K:181:PHE:H | 1.73 | 0.53 |
| 5:J:326:MET:HE1 | 5:K:264:ARG:H | 1.72 | 0.53 |
| 5:J:465:ASN:ND2 | 5:K:418:GLY:O | 2.42 | 0.53 |
| 6:M:10:VAL:HG22 | 6:N:13:ARG:HB2 | 1.91 | 0.53 |
| 6:M:135:GLU:HA | 6:M:138:ALA:HB3 | 1.89 | 0.53 |
| 6:N:100:PRO:O | 6:N:103:SER:OG | 2.18 | 0.53 |
| 7:O:231:GLY:HA2 | 7:P:222:GLU:HG3 | 1.89 | 0.53 |
| 7:O:45:ASN:CG | 7:P:24:ASN:HD21 | 2.13 | 0.53 |
| 7:O:59:PHE:CZ | 7:P:55:LYS:HG3 | 2.44 | 0.53 |
| 7:O:265:LEU:O | 7:P:257:THR:HA | 2.08 | 0.53 |
| 7:Q:372:CYS:SG | 7:Q:525:VAL:HB | 2.49 | 0.53 |
| 10:U:205:LYS:HB2 | 10:U:311:PHE:HZ | 1.74 | 0.53 |
| 1:X:80:MET:HG3 | 1:X:81:ARG:HG3 | 1.90 | 0.53 |
| 13:YA:18[F]:ARG:NH1 | 13:YA:77[F]:VAL:HG23 | 2.23 | 0.53 |
| 13:YA:193[D]:ASP:OD1 | 13:YA:197[D]:TYR:N | 2.33 | 0.53 |
| 13:YA:256[E]:ILE:HA | 13:YA:286[E]:VAL:HG21 | 1.91 | 0.53 |
| 13:YA:425[A]:SER:HB2 | 13:YA:426[A]:PRO:HD2 | 1.89 | 0.53 |
| 13:YA:437[A]:ASN:HB3 | 13:YA:439[A]:TYR:CE1 | 2.43 | 0.53 |
| 13:YA:466[B]:ASN:HB2 | 13:YC:474[B]:ILE:HG12 | 1.89 | 0.53 |
| 13:YA:481[E]:PHE:O | 13:YB:473[E]:GLN:HA | 2.09 | 0.53 |
| 13:YA:495[F]:THR:HA | 13:YC:503[F]:THR:O | 2.08 | 0.53 |
| 13:YB:148[C]:GLN:OE1 | 13:YB:381[C]:SER:HB2 | 2.09 | 0.53 |
| 13:YB:460[F]:GLY:N | 13:YC:452[F]:GLY:O | 2.42 | 0.53 |
| 13:YC:26[C]:ARG:HA | 13:YC:55[C]:MET:O | 2.08 | 0.53 |
| 13:YC:148[B]:GLN:OE1 | 13:YC:381[B]:SER:HB2 | 2.09 | 0.53 |
| 13:YC:16[A]:GLU:OE2 | 13:YC:39[A]:ARG:NH2 | 2.42 | 0.53 |
| 13:YC:57[F]:VAL:HG11 | 13:YC:76[F]:PRO:HD3 | 1.91 | 0.53 |
| 14:YD:232[F]:TYR:HD2 | 14:YD:233[F]:ASP:OD1 | 1.92 | 0.53 |
| 14:YD:238[A]:THR:OG1 | 14:YE:92[A]:HIS:NE2 | 2.42 | 0.53 |
| 14:YD:73[A]:SER:OG | 14:YD:85[A]:THR:OG1 | 2.27 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:232[C]:TYR:HD2 | 14:YE:233[C]:ASP:OD1 | 1.92 | 0.53 |
| 14:YD:238[E]:THR:OG1 | 14:YE:92[E]:HIS:NE2 | 2.42 | 0.53 |
| 14:YF:16[A]:LEU:HA | 14:YF:69[A]:ILE:O | 2.08 | 0.53 |
| 14:YF:16[F]:LEU:HA | 14:YF:69[F]:ILE:O | 2.08 | 0.53 |
| 14:YF:73[B]:SER:OG | 14:YF:85[B]:THR:OG1 | 2.27 | 0.53 |
| 2:Z:446:SER:HB2 | 2:Z:485:TYR:OH | 2.09 | 0.53 |
| 2:Z:544:VAL:HG12 | 2:Z:546:GLU:HB3 | 1.90 | 0.53 |
| 15:ZA:2[C]:SER:N | 15:ZA:96[C]:ILE:O | 2.42 | 0.53 |
| 1:A:642:PHE:CZ | 1:A:644:ASN:HB2 | 2.44 | 0.53 |
| 4:AB:131:LYS:HD2 | 4:AB:151:ILE:HD13 | 1.91 | 0.53 |
| 5:AD:465:ASN:ND2 | 5:AE:418:GLY:O | 2.42 | 0.53 |
| 7:AI:66:VAL:HG21 | 7:AI:80:THR:HB | 1.91 | 0.53 |
| 7:AJ:325:TYR:CD1 | 7:AJ:330:ARG:HA | 2.41 | 0.53 |
| 1:B:103:LYS:N | 1:B:319:PRO:HB3 | 2.24 | 0.53 |
| 1:B:555:ILE:O | 1:B:589:TYR:HD1 | 1.92 | 0.53 |
| 7:AI:512:THR:O | 7:BA:514:PRO:HB3 | 2.09 | 0.53 |
| 1:BH:299:ASN:OD1 | 1:BH:300:ILE:N | 2.42 | 0.53 |
| 1:BH:80:MET:HG3 | 1:BH:81:ARG:HG3 | 1.90 | 0.53 |
| 2:BJ:138:ASN:OD1 | 2:BJ:139:ASN:ND2 | 2.42 | 0.53 |
| 2:BJ:191:TYR:HE1 | 2:BJ:235:LYS:HA | 1.73 | 0.53 |
| 2:BJ:339:ASP:HB3 | 2:BJ:340:PRO:CD | 2.36 | 0.53 |
| 2:BJ:919:TYR:HA | 2:BJ:990:MET:HE3 | 1.90 | 0.53 |
| 2:C:446:SER:HB2 | 2:C:485:TYR:OH | 2.09 | 0.53 |
| 2:C:646:ARG:CD | 2:C:673:GLN:HE22 | 2.13 | 0.53 |
| 2:C:934:ALA:HB1 | 2:C:942:ILE:HD12 | 1.91 | 0.53 |
| 4:CE:161:ASN:OD1 | 4:CE:162:TYR:N | 2.41 | 0.53 |
| 4:CD:172:GLU:HA | 4:CE:166:SER:H | 1.73 | 0.53 |
| 5:CH:398:GLU:N | 5:CH:398:GLU:OE1 | 2.37 | 0.53 |
| 6:CI:135:GLU:HA | 6:CI:138:ALA:HB3 | 1.90 | 0.53 |
| 7:DB:476:ASP:OD2 | 7:DC:454:HIS:HE1 | 1.92 | 0.53 |
| 7:DB:73:THR:HG23 | 7:DB:74:LYS:H | 1.73 | 0.53 |
| 7:DC:325:TYR:CD1 | 7:DC:330:ARG:HA | 2.41 | 0.53 |
| 7:DD:233:GLN:HE21 | 7:DD:237:ASN:HD21 | 1.56 | 0.53 |
| 7:DB:315:ILE:HG12 | 7:DD:308:ILE:HD12 | 1.91 | 0.53 |
| 9:DG:87:ARG:O | 9:DG:113:ILE:HG12 | 2.09 | 0.53 |
| 12:BG:251:GLY:HA3 | 12:DJ:104:PHE:CG | 2.44 | 0.53 |
| 3:E:122:THR:HG22 | 3:E:169:PRO:HG2 | 1.91 | 0.53 |
| 1:EA:231:ASP:OD1 | 1:EA:233:ASN:N | 2.36 | 0.53 |
| 1:EA:238:PHE:HE1 | 1:EA:262:PRO:HD2 | 1.73 | 0.53 |
| 1:EA:45:ASP:OD1 | 1:EA:46:TYR:N | 2.41 | 0.53 |
| 1:EA:80:MET:HG3 | 1:EA:81:ARG:HG3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:448:TYR:CD1 | 1:EB:452:VAL:HG11 | 2.44 | 0.53 |
| 2:EC:177:GLN:HG3 | 2:EC:215:LYS:HB2 | 1.90 | 0.53 |
| 2:EC:205:TYR:HB2 | 2:EC:206:GLN:OE1 | 2.09 | 0.53 |
| 2:EC:450:PHE:HZ | 2:EC:473:TYR:HE1 | 1.56 | 0.53 |
| 2:EC:39:ALA:HB2 | 2:EC:56:TRP:CZ3 | 2.44 | 0.53 |
| 3:EE:150:LYS:HB2 | 3:EE:160:TRP:CE2 | 2.44 | 0.53 |
| 5:EI:258:TYR:HE1 | 5:EI:384:THR:HG23 | 1.74 | 0.53 |
| 5:EI:362:GLU:HB3 | 5:EI:367:GLU:OE1 | 2.08 | 0.53 |
| 5:EJ:186:TYR:OH | 5:EJ:191:ILE:HA | 2.09 | 0.53 |
| 5:EJ:196:ARG:HE | 7:FG:5:THR:HG23 | 1.74 | 0.53 |
| 5:EJ:65:GLY:O | 5:FA:45:SER:OG | 2.14 | 0.53 |
| 6:FC:135:GLU:HA | 6:FC:138:ALA:HB3 | 1.89 | 0.53 |
| 8:FH:17:ARG:NH2 | 8:FH:118:ARG:HD3 | 2.23 | 0.53 |
| 8:FI:82:ARG:HH12 | 8:FI:138:GLY:HA2 | 1.73 | 0.53 |
| 9:FJ:100:ASP:OD1 | 9:FJ:101:ASP:N | 2.34 | 0.53 |
| 4:G:111:ASN:HD21 | 4:G:116:ILE:H | 1.56 | 0.53 |
| 11:GB:54:PRO:HG2 | 11:GB:59:LEU:HB2 | 1.90 | 0.53 |
| 1:GE:433:GLU:O | 1:GE:436:LEU:N | 2.42 | 0.53 |
| 2:GF:494:GLU:HG3 | 2:GF:498:TRP:CD2 | 2.44 | 0.53 |
| 5:HB:258:TYR:HE1 | 5:HB:384:THR:HG23 | 1.74 | 0.53 |
| 5:HD:186:TYR:OH | 5:HD:190:ASN:O | 2.12 | 0.53 |
| 5:HD:212:PHE:HZ | 5:HD:230:ILE:HB | 1.74 | 0.53 |
| 5:HD:54:ALA:HB2 | 5:HD:71:ASN:O | 2.09 | 0.53 |
| 7:HJ:123:VAL:O | 7:HJ:127:ASN:N | 2.26 | 0.53 |
| 7:HH:56:GLY:CA | 7:HJ:57:ILE:HG23 | 2.39 | 0.53 |
| 5:I:264:ARG:HA | 5:I:379:ASP:O | 2.09 | 0.53 |
| 5:I:49:TRP:CD1 | 5:I:67:SER:HB3 | 2.44 | 0.53 |
| 8:IB:67:ASP:OD1 | 8:IB:68:ASP:N | 2.42 | 0.53 |
| 5:J:358:VAL:HG22 | 5:J:371:PHE:HB2 | 1.89 | 0.53 |
| 5:J:90:ASN:HA | 5:K:98:VAL:HG22 | 1.91 | 0.53 |
| 5:K:206:PHE:CD2 | 5:K:223:VAL:HA | 2.44 | 0.53 |
| 8:R:82:ARG:HH12 | 8:R:138:GLY:HA2 | 1.73 | 0.53 |
| 12:W:126:TYR:CD2 | 12:W:163:ARG:HG3 | 2.44 | 0.53 |
| 1:X:45:ASP:OD1 | 1:X:46:TYR:N | 2.41 | 0.53 |
| 1:Y:236:PHE:CE2 | 1:Y:270:ILE:HD11 | 2.44 | 0.53 |
| 13:YB:148[A]:GLN:OE1 | 13:YB:381[A]:SER:HB2 | 2.09 | 0.53 |
| 13:YA:442[A]:THR:HA | 13:YB:434[A]:THR:O | 2.09 | 0.53 |
| 13:YA:442[C]:THR:HA | 13:YB:434[C]:THR:O | 2.09 | 0.53 |
| 13:YA:454[A]:LYS:NZ | 13:YB:464[A]:TYR:OH | 2.42 | 0.53 |
| 13:YB:527[D]:THR:O | 13:YC:519[D]:THR:HA | 2.08 | 0.53 |
| 13:YC:148[A]:GLN:OE1 | 13:YC:381[A]:SER:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:148[E]:GLN:OE1 | 13:YC:381[E]:SER:HB2 | 2.09 | 0.53 |
| 13:YC:76[C]:PRO:C | 13:YC:98[C]:GLY:HA2 | 2.29 | 0.53 |
| 14:YD:123[A]:PRO:HA | 14:YD:161[A]:PRO:HA | 1.90 | 0.53 |
| 14:YD:73[E]:SER:OG | 14:YD:85[E]:THR:OG1 | 2.27 | 0.53 |
| 14:YE:16[B]:LEU:HA | 14:YE:69[B]:ILE:O | 2.08 | 0.53 |
| 2:Z:408:HIS:ND1 | 2:Z:410:GLU:OE2 | 2.42 | 0.53 |
| 2:Z:326:VAL:HG11 | 2:Z:413:TRP:CZ2 | 2.44 | 0.53 |
| 2:Z:555:ARG:HD3 | 2:Z:557:VAL:HB | 1.90 | 0.53 |
| 2:Z:788:THR:HG23 | 2:Z:790:THR:N | 2.24 | 0.53 |
| 15:ZA:76[B]:GLN:HB3 | 15:ZA:96[B]:ILE:HD11 | 1.91 | 0.53 |
| 5:AC:340:VAL:HG21 | 6:AG:174:TYR:H | 1.74 | 0.52 |
| 5:AC:362:GLU:HB3 | 5:AC:367:GLU:OE1 | 2.08 | 0.52 |
| 5:AD:86:VAL:HG22 | 5:AD:87:ASN:H | 1.75 | 0.52 |
| 7:AJ:110:VAL:HG12 | 7:AJ:111:ASN:H | 1.74 | 0.52 |
| 7:AJ:20:PRO:HG3 | 7:AJ:29:ILE:HG13 | 1.91 | 0.52 |
| 7:BA:372:CYS:SG | 7:BA:525:VAL:HB | 2.48 | 0.52 |
| 8:BB:5:ASP:OD1 | 8:BB:8:ARG:NH1 | 2.42 | 0.52 |
| 11:BF:36:PHE:HZ | 11:BF:76:CYS:HG | 1.55 | 0.52 |
| 1:BI:103:LYS:N | 1:BI:319:PRO:HB3 | 2.24 | 0.52 |
| 2:BJ:107:ALA:HB2 | 2:BJ:128:THR:HA | 1.91 | 0.52 |
| 2:BJ:4:LYS:HA | 2:BJ:90:GLU:HB3 | 1.91 | 0.52 |
| 2:BJ:788:THR:HG23 | 2:BJ:790:THR:N | 2.24 | 0.52 |
| 2:C:39:ALA:HB2 | 2:C:56:TRP:CZ3 | 2.44 | 0.52 |
| 3:CB:150:LYS:HB2 | 3:CB:160:TRP:CE2 | 2.44 | 0.52 |
| 5:CF:117:ILE:HG13 | 5:CF:118:LYS:H | 1.73 | 0.52 |
| 5:CF:72:THR:HG22 | 5:CF:77:VAL:HG22 | 1.91 | 0.52 |
| 5:CH:186:TYR:HB3 | 5:CH:227:GLY:O | 2.08 | 0.52 |
| 5:CH:54:ALA:HB2 | 5:CH:71:ASN:O | 2.09 | 0.52 |
| 7:DC:110:VAL:HG12 | 7:DC:111:ASN:H | 1.75 | 0.52 |
| 7:DD:34:ALA:HA | 7:DD:37:ALA:HB3 | 1.91 | 0.52 |
| 1:EA:187:ILE:HD11 | 1:EA:270:ILE:HD13 | 1.91 | 0.52 |
| 1:EA:53:LEU:HB2 | 9:FJ:23:VAL:HG23 | 1.90 | 0.52 |
| 2:EC:138:ASN:OD1 | 2:EC:139:ASN:ND2 | 2.42 | 0.52 |
| 4:EG:111:ASN:OD1 | 4:EG:114:GLY:N | 2.41 | 0.52 |
| 5:EJ:132:ASP:HB2 | 5:EJ:149:LYS:HG3 | 1.91 | 0.52 |
| 7:FE:146:SER:HB3 | 7:FE:148:PRO:HD2 | 1.91 | 0.52 |
| 7:FE:297:TYR:HB2 | 7:FG:291:ARG:HA | 1.90 | 0.52 |
| 7:FE:90:ALA:HB2 | 7:FE:96:GLY:N | 2.24 | 0.52 |
| 7:FG:176:ILE:HG23 | 7:FG:177:ALA:H | 1.73 | 0.52 |
| 4:G:27:GLY:HA2 | 4:G:30:LYS:HD2 | 1.91 | 0.52 |
| 10:GA:286:VAL:HG22 | 10:GA:287:VAL:H | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:GC:125:ILE:HA | 12:GC:162:PHE:CB | 2.39 | 0.52 |
| 1:GD:485:VAL:HG22 | 1:GD:624:TYR:HD1 | 1.72 | 0.52 |
| 1:GE:348:PHE:CZ | 1:GE:399:TYR:HD2 | 2.28 | 0.52 |
| 2:GF:544:VAL:HG12 | 2:GF:546:GLU:HB3 | 1.90 | 0.52 |
| 2:GF:39:ALA:HB2 | 2:GF:56:TRP:CZ3 | 2.44 | 0.52 |
| 2:GF:7:SER:O | 2:GF:28:VAL:HG11 | 2.09 | 0.52 |
| 2:GF:919:TYR:HA | 2:GF:990:MET:HE3 | 1.90 | 0.52 |
| 3:GH:150:LYS:HB2 | 3:GH:160:TRP:CE2 | 2.44 | 0.52 |
| 4:GI:27:GLY:HA2 | 4:GI:30:LYS:HD2 | 1.91 | 0.52 |
| 4:GJ:111:ASN:HD21 | 4:GJ:116:ILE:H | 1.56 | 0.52 |
| 4:H:111:ASN:HD21 | 4:H:116:ILE:H | 1.56 | 0.52 |
| 5:HB:319:GLU:OE2 | 5:HB:324:VAL:HG13 | 2.08 | 0.52 |
| 5:HB:407:TYR:OH | 5:HD:403:THR:HA | 2.09 | 0.52 |
| 5:HB:64:TRP:CE2 | 5:HB:82:PRO:HG2 | 2.44 | 0.52 |
| 5:HC:85:THR:HB | 5:HC:137:TYR:CE2 | 2.44 | 0.52 |
| 2:GF:206:GLN:HG3 | 5:HD:555:CYS:O | 2.09 | 0.52 |
| 7:Q:365:GLY:HA2 | 7:HI:71:ASN:CG | 2.29 | 0.52 |
| 7:HJ:173:ILE:O | 7:HJ:178:PRO:HD2 | 2.09 | 0.52 |
| 5:I:258:TYR:HE1 | 5:I:384:THR:HG23 | 1.74 | 0.52 |
| 5:I:469:PRO:HB2 | 5:I:478:TRP:CD1 | 2.44 | 0.52 |
| 5:I:552:VAL:HG11 | 5:K:569:TYR:CE2 | 2.44 | 0.52 |
| 8:S:79:HIS:HE2 | 8:IB:115:GLN:HG2 | 1.74 | 0.52 |
| 8:IB:5:ASP:OD1 | 8:IB:8:ARG:NH1 | 2.43 | 0.52 |
| 10:ID:285:LEU:HA | 14:YD:215[F]:GLU:HG2 | 1.90 | 0.52 |
| 12:IF:125:ILE:HA | 12:IF:162:PHE:CB | 2.39 | 0.52 |
| 5:J:89:TYR:CE1 | 5:J:139:ALA:HA | 2.45 | 0.52 |
| 5:J:186:TYR:OH | 5:J:191:ILE:HA | 2.09 | 0.52 |
| 5:J:501:LEU:HB3 | 5:J:512:PRO:HB2 | 1.91 | 0.52 |
| 5:J:85:THR:HB | 5:J:137:TYR:CE2 | 2.44 | 0.52 |
| 5:J:98:VAL:CG1 | 5:J:99:PHE:HD2 | 2.21 | 0.52 |
| 5:K:166:GLU:OE1 | 5:K:166:GLU:N | 2.42 | 0.52 |
| 7:O:322:THR:HG23 | 7:P:327:GLN:HE21 | 1.75 | 0.52 |
| 7:P:349:TRP:N | 7:P:520:ASN:O | 2.38 | 0.52 |
| 7:Q:289:GLN:OE1 | 7:Q:294:GLN:NE2 | 2.40 | 0.52 |
| 7:P:341:ILE:HG13 | 7:Q:341:ILE:HD11 | 1.90 | 0.52 |
| 8:S:36:CYS:HA | 8:S:73:VAL:HG12 | 1.91 | 0.52 |
| 9:T:87:ARG:O | 9:T:113:ILE:HG12 | 2.09 | 0.52 |
| 11:V:186:ARG:CG | 11:V:187:ILE:HG12 | 2.35 | 0.52 |
| 13:YA:25[E]:GLY:HA3 | 13:YA:73[E]:VAL:HG12 | 1.90 | 0.52 |
| 13:YA:26[C]:ARG:HA | 13:YA:55[C]:MET:O | 2.08 | 0.52 |
| 13:YA:270[E]:ASN:O | 13:YA:274[E]:GLN:N | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:256[B]:ILE:HA | 13:YA:286[B]:VAL:HG21 | 1.91 | 0.52 |
| 13:YA:148[D]:GLN:OE1 | 13:YA:381[D]:SER:HB2 | 2.09 | 0.52 |
| 13:YA:16[A]:GLU:OE2 | 13:YA:39[A]:ARG:NH2 | 2.42 | 0.52 |
| 13:YA:18[A]:ARG:NH1 | 13:YA:77[A]:VAL:HG23 | 2.23 | 0.52 |
| 13:YA:9[D]:ASN:HA | 13:YC:7[D]:ASN:ND2 | 2.17 | 0.52 |
| 13:YB:148[B]:GLN:OE1 | 13:YB:381[B]:SER:HB2 | 2.09 | 0.52 |
| 13:YB:270[C]:ASN:O | 13:YB:274[C]:GLN:N | 2.42 | 0.52 |
| 13:YB:538[E]:VAL:HG11 | 13:YC:534[E]:LEU:CB | 2.38 | 0.52 |
| 13:YC:148[D]:GLN:OE1 | 13:YC:381[D]:SER:HB2 | 2.09 | 0.52 |
| 13:YC:256[A]:ILE:HA | 13:YC:286[A]:VAL:HG21 | 1.92 | 0.52 |
| 13:YA:461[C]:SER:OG | 13:YC:468[C]:ASP:OD2 | 2.27 | 0.52 |
| 13:YB:527[E]:THR:O | 13:YC:519[E]:THR:HA | 2.08 | 0.52 |
| 13:YA:520[E]:THR:O | 13:YC:529[E]:THR:N | 2.42 | 0.52 |
| 13:YA:565[C]:TYR:CE2 | 13:YC:567[C]:ILE:HG23 | 2.44 | 0.52 |
| 13:YA:565[D]:TYR:CE2 | 13:YC:567[D]:ILE:HG23 | 2.44 | 0.52 |
| 14:YE:73[F]:SER:OG | 14:YE:85[F]:THR:OG1 | 2.27 | 0.52 |
| 14:YF:232[B]:TYR:HD2 | 14:YF:233[B]:ASP:OD1 | 1.92 | 0.52 |
| 14:YF:232[D]:TYR:HD2 | 14:YF:233[D]:ASP:OD1 | 1.92 | 0.52 |
| 5:AC:206:PHE:CG | 5:AC:223:VAL:HA | 2.44 | 0.52 |
| 5:AC:208:GLU:OE1 | 5:AC:233:ARG:NH2 | 2.43 | 0.52 |
| 5:AC:49:TRP:CD1 | 5:AC:67:SER:HB3 | 2.44 | 0.52 |
| 5:AC:72:THR:HG22 | 5:AC:77:VAL:HG22 | 1.91 | 0.52 |
| 5:AD:323:THR:CG2 | 5:AD:359:GLU:HB2 | 2.39 | 0.52 |
| 5:AC:484:GLY:N | 5:AD:489:GLY:O | 2.29 | 0.52 |
| 5:AE:20:ARG:HH12 | 5:AE:24:ILE:HD12 | 1.73 | 0.52 |
| 5:AE:313:PHE:CD2 | 5:AE:320:LEU:HD21 | 2.44 | 0.52 |
| 1:B:209:TRP:HB2 | 1:B:225:TYR:HE1 | 1.75 | 0.52 |
| 7:BA:173:ILE:O | 7:BA:178:PRO:HD2 | 2.09 | 0.52 |
| 7:AJ:210:ILE:O | 7:BA:210:ILE:HG22 | 2.09 | 0.52 |
| 9:BD:61:LEU:HG | 9:BD:69:THR:HG23 | 1.91 | 0.52 |
| 1:BH:286:PHE:HB2 | 1:BH:300:ILE:CD1 | 2.39 | 0.52 |
| 1:BI:448:TYR:CD1 | 1:BI:452:VAL:HG11 | 2.44 | 0.52 |
| 1:BI:519:SER:HB3 | 1:BI:533:ASP:OD2 | 2.09 | 0.52 |
| 1:BI:83:ALA:O | 1:BI:326:ARG:NH2 | 2.36 | 0.52 |
| 2:BJ:180:ILE:HA | 2:BJ:219:TRP:CH2 | 2.45 | 0.52 |
| 2:BJ:380:ILE:O | 2:BJ:401:LYS:HD2 | 2.10 | 0.52 |
| 2:BJ:575:PHE:O | 2:BJ:607:THR:OG1 | 2.13 | 0.52 |
| 2:C:494:GLU:HG3 | 2:C:498:TRP:CD2 | 2.44 | 0.52 |
| 3:CA:43:ARG:H | 3:CA:74:HIS:HB3 | 1.73 | 0.52 |
| 3:CB:202:ARG:O | 3:CB:248:ARG:NH1 | 2.42 | 0.52 |
| 4:CC:201:LYS:HB3 | 4:CC:280:ALA:HB3 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CD:240:VAL:HG22 | 4:CE:231:ILE:HD13 | 1.91 | 0.52 |
| 5:CF:469:PRO:HB2 | 5:CF:478:TRP:CD1 | 2.44 | 0.52 |
| 5:CF:78:THR:HA | 5:CF:108:THR:HB | 1.90 | 0.52 |
| 5:CG:186:TYR:OH | 5:CG:191:ILE:HA | 2.09 | 0.52 |
| 7:DB:90:ALA:HB2 | 7:DB:96:GLY:N | 2.24 | 0.52 |
| 8:BC:9:ALA:HB2 | 8:DF:34:PHE:HD2 | 1.74 | 0.52 |
| 9:DG:65:MET:SD | 9:DG:97:PRO:HB2 | 2.48 | 0.52 |
| 3:E:150:LYS:HB2 | 3:E:160:TRP:CE2 | 2.44 | 0.52 |
| 2:EC:380:ILE:O | 2:EC:401:LYS:HD2 | 2.10 | 0.52 |
| 2:EC:91:GLN:NE2 | 2:EC:92:SER:H | 2.06 | 0.52 |
| 4:EG:79:VAL:N | 4:EG:97:ILE:O | 2.31 | 0.52 |
| 5:EJ:117:ILE:HG22 | 5:EJ:143:TRP:CE3 | 2.42 | 0.52 |
| 4:F:111:ASN:HD21 | 4:F:116:ILE:H | 1.56 | 0.52 |
| 4:F:161:ASN:OD1 | 4:F:162:TYR:N | 2.41 | 0.52 |
| 5:FA:166:GLU:N | 5:FA:166:GLU:OE1 | 2.42 | 0.52 |
| 5:FA:323:THR:HG21 | 5:FA:354:THR:HG23 | 1.91 | 0.52 |
| 6:FC:195:LEU:HD13 | 6:FC:215:PHE:HE1 | 1.74 | 0.52 |
| 7:FE:73:THR:HG23 | 7:FE:74:LYS:H | 1.73 | 0.52 |
| 7:FE:66:VAL:HG21 | 7:FE:80:THR:HB | 1.91 | 0.52 |
| 7:FF:47:VAL:HG12 | 7:FF:48:PRO:N | 2.24 | 0.52 |
| 9:FJ:61:LEU:HG | 9:FJ:69:THR:HG23 | 1.91 | 0.52 |
| 4:G:240:VAL:HG22 | 4:H:231:ILE:HD13 | 1.91 | 0.52 |
| 1:GE:103:LYS:N | 1:GE:319:PRO:HB3 | 2.24 | 0.52 |
| 1:GE:517:PHE:N | 1:GE:536:TYR:O | 2.43 | 0.52 |
| 2:GF:193:MET:HG3 | 2:GF:238:TYR:CE1 | 2.44 | 0.52 |
| 2:GF:417:PHE:CZ | 2:GF:423:GLU:HB3 | 2.44 | 0.52 |
| 2:GF:4:LYS:HA | 2:GF:90:GLU:HB3 | 1.91 | 0.52 |
| 2:EC:449:LYS:HD2 | 3:GG:74:HIS:CE1 | 2.43 | 0.52 |
| 4:GI:161:ASN:OD1 | 4:GI:162:TYR:N | 2.41 | 0.52 |
| 4:H:124:ILE:HD12 | 4:H:137:LEU:HD23 | 1.90 | 0.52 |
| 4:HA:79:VAL:N | 4:HA:97:ILE:O | 2.32 | 0.52 |
| 5:HC:117:ILE:HG22 | 5:HC:143:TRP:CE3 | 2.42 | 0.52 |
| 5:HC:132:ASP:HB2 | 5:HC:149:LYS:HG3 | 1.91 | 0.52 |
| 5:HB:201:TYR:HB3 | 5:HC:166:GLU:HG2 | 1.90 | 0.52 |
| 5:HC:186:TYR:OH | 5:HC:191:ILE:HA | 2.09 | 0.52 |
| 5:HC:326:MET:HE1 | 5:HD:264:ARG:H | 1.74 | 0.52 |
| 7:HH:49:ASP:O | 7:HH:56:GLY:HA3 | 2.09 | 0.52 |
| 7:HI:110:VAL:HG12 | 7:HI:111:ASN:H | 1.74 | 0.52 |
| 5:I:257:SER:OG | 5:I:387:ASN:HB2 | 2.10 | 0.52 |
| 5:I:67:SER:HB2 | 5:I:94:ARG:HB2 | 1.91 | 0.52 |
| 5:J:204:ASP:OD1 | 5:J:205:VAL:N | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:305:ASN:OD1 | 5:K:305:ASN:N | 2.42 | 0.52 |
| 5:K:323:THR:HG21 | 5:K:354:THR:HG23 | 1.91 | 0.52 |
| 6:L:195:LEU:HD13 | 6:L:215:PHE:HE1 | 1.74 | 0.52 |
| 7:O:383:TYR:CD1 | 7:O:393:PRO:HG3 | 2.44 | 0.52 |
| 7:O:216:MET:SD | 7:P:202:GLY:HA3 | 2.49 | 0.52 |
| 7:P:394:ASP:OD2 | 7:Q:407:SER:N | 2.30 | 0.52 |
| 7:P:447:HIS:CD2 | 7:Q:447:HIS:CD2 | 2.97 | 0.52 |
| 7:O:439:ILE:HG23 | 7:Q:515:TRP:CZ2 | 2.44 | 0.52 |
| 8:R:5:ASP:OD1 | 8:R:8:ARG:NH1 | 2.42 | 0.52 |
| 12:W:104:PHE:CG | 12:IF:251:GLY:HA3 | 2.44 | 0.52 |
| 1:X:447:TYR:HB2 | 1:X:467:TYR:HD2 | 1.73 | 0.52 |
| 1:Y:348:PHE:CZ | 1:Y:399:TYR:HD2 | 2.27 | 0.52 |
| 13:YA:148[E]:GLN:OE1 | 13:YA:381[E]:SER:HB2 | 2.09 | 0.52 |
| 13:YA:454[C]:LYS:NZ | 13:YB:464[C]:TYR:OH | 2.41 | 0.52 |
| 13:YA:71[F]:GLY:HA2 | 13:YB:393[F]:MET:HA | 1.91 | 0.52 |
| 13:YB:148[E]:GLN:OE1 | 13:YB:381[E]:SER:HB2 | 2.09 | 0.52 |
| 13:YA:481[A]:PHE:O | 13:YB:473[A]:GLN:HA | 2.09 | 0.52 |
| 13:YC:148[C]:GLN:OE1 | 13:YC:381[C]:SER:HB2 | 2.09 | 0.52 |
| 13:YC:148[F]:GLN:OE1 | 13:YC:381[F]:SER:HB2 | 2.09 | 0.52 |
| 13:YC:256[D]:ILE:HA | 13:YC:286[D]:VAL:HG21 | 1.92 | 0.52 |
| 13:YB:554[C]:MET:HG3 | 13:YC:550[C]:TRP:HB2 | 1.91 | 0.52 |
| 14:YD:238[F]:THR:OG1 | 14:YE:92[F]:HIS:NE2 | 2.43 | 0.52 |
| 14:YE:73[C]:SER:OG | 14:YE:85[C]:THR:OG1 | 2.27 | 0.52 |
| 14:YF:73[E]:SER:OG | 14:YF:85[E]:THR:OG1 | 2.27 | 0.52 |
| 2:Z:39:ALA:HB2 | 2:Z:56:TRP:CZ3 | 2.44 | 0.52 |
| 1:A:447:TYR:HB2 | 1:A:467:TYR:HD2 | 1.73 | 0.52 |
| 5:AC:258:TYR:HE1 | 5:AC:384:THR:HG23 | 1.74 | 0.52 |
| 5:AC:560:ASP:HB3 | 5:AC:561:GLU:OE1 | 2.09 | 0.52 |
| 5:AD:85:THR:HB | 5:AD:137:TYR:CE2 | 2.44 | 0.52 |
| 5:AD:196:ARG:NE | 7:BA:5:THR:HG23 | 2.23 | 0.52 |
| 5:AE:193:VAL:O | 5:AE:199:GLU:N | 2.38 | 0.52 |
| 5:AC:255:ARG:NH2 | 5:AE:390:LEU:HB2 | 2.24 | 0.52 |
| 7:AI:146:SER:O | 7:AI:150:ALA:N | 2.38 | 0.52 |
| 1:B:189:ASP:HA | 11:V:121:TYR:CE2 | 2.44 | 0.52 |
| 1:B:348:PHE:CZ | 1:B:399:TYR:HD2 | 2.27 | 0.52 |
| 8:BB:67:ASP:OD1 | 8:BB:68:ASP:N | 2.42 | 0.52 |
| 12:BG:126:TYR:CD2 | 12:BG:163:ARG:HG3 | 2.44 | 0.52 |
| 2:BJ:299:THR:O | 2:BJ:349:LEU:HD22 | 2.09 | 0.52 |
| 2:BJ:406:LEU:HD11 | 2:BJ:413:TRP:HA | 1.89 | 0.52 |
| 2:BJ:450:PHE:CZ | 2:BJ:473:TYR:HE1 | 2.27 | 0.52 |
| 2:BJ:703:TYR:OH | 2:BJ:725:ARG:NH1 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:703:TYR:OH | 2:C:725:ARG:NH1 | 2.43 | 0.52 |
| 5:CF:208:GLU:OE1 | 5:CF:233:ARG:NH2 | 2.42 | 0.52 |
| 5:CF:264:ARG:HA | 5:CF:379:ASP:O | 2.09 | 0.52 |
| 5:CF:362:GLU:HB3 | 5:CF:367:GLU:OE1 | 2.08 | 0.52 |
| 5:CF:92:VAL:HG12 | 5:CF:136:VAL:HG12 | 1.91 | 0.52 |
| 5:CH:102:TRP:HB2 | 5:CH:129:ARG:O | 2.10 | 0.52 |
| 5:CH:305:ASN:OD1 | 5:CH:305:ASN:N | 2.42 | 0.52 |
| 5:CH:313:PHE:CD2 | 5:CH:320:LEU:HD21 | 2.44 | 0.52 |
| 5:CH:356:TYR:HE1 | 6:CJ:4:LEU:HD13 | 1.75 | 0.52 |
| 5:CF:255:ARG:NH2 | 5:CH:390:LEU:HB2 | 2.25 | 0.52 |
| 9:DG:61:LEU:HG | 9:DG:69:THR:HG23 | 1.91 | 0.52 |
| 12:DJ:23:SER:N | 12:DJ:202:ASN:O | 2.29 | 0.52 |
| 2:EC:180:ILE:HA | 2:EC:219:TRP:CH2 | 2.45 | 0.52 |
| 2:EC:206:GLN:C | 2:EC:208:VAL:H | 2.13 | 0.52 |
| 2:EC:7:SER:O | 2:EC:28:VAL:HG11 | 2.09 | 0.52 |
| 2:EC:299:THR:O | 2:EC:349:LEU:HD22 | 2.09 | 0.52 |
| 4:EG:131:LYS:N | 4:EG:160:TRP:O | 2.29 | 0.52 |
| 5:FA:107:VAL:O | 5:FA:125:GLU:HG3 | 2.09 | 0.52 |
| 5:FA:186:TYR:HB3 | 5:FA:227:GLY:O | 2.08 | 0.52 |
| 5:FA:313:PHE:CD2 | 5:FA:320:LEU:HD21 | 2.44 | 0.52 |
| 7:FE:231:GLY:HA2 | 7:FF:222:GLU:HG3 | 1.92 | 0.52 |
| 7:FF:99:ARG:HD3 | 7:FF:111:ASN:ND2 | 2.20 | 0.52 |
| 8:FH:5:ASP:OD1 | 8:FH:8:ARG:NH1 | 2.43 | 0.52 |
| 8:FH:36:CYS:HA | 8:FH:73:VAL:HG12 | 1.91 | 0.52 |
| 1:GD:238:PHE:HE1 | 1:GD:262:PRO:HD2 | 1.73 | 0.52 |
| 1:GD:299:ASN:OD1 | 1:GD:300:ILE:N | 2.42 | 0.52 |
| 2:GF:446:SER:HB2 | 2:GF:485:TYR:OH | 2.09 | 0.52 |
| 2:GF:174:HIS:CG | 2:GF:508:TYR:HH | 2.27 | 0.52 |
| 3:GH:232:GLN:O | 3:GH:232:GLN:HG2 | 2.10 | 0.52 |
| 4:GI:131:LYS:HD2 | 4:GI:151:ILE:HD13 | 1.91 | 0.52 |
| 4:GJ:131:LYS:HD2 | 4:GJ:151:ILE:HD13 | 1.91 | 0.52 |
| 5:HB:98:VAL:HG11 | 5:HD:89:TYR:HB3 | 1.91 | 0.52 |
| 5:HC:89:TYR:CE1 | 5:HC:139:ALA:HA | 2.44 | 0.52 |
| 5:HD:166:GLU:OE1 | 5:HD:166:GLU:N | 2.42 | 0.52 |
| 5:HD:357:SER:OG | 6:HF:4:LEU:HD21 | 2.09 | 0.52 |
| 7:HH:73:THR:HG23 | 7:HH:74:LYS:H | 1.73 | 0.52 |
| 7:HH:78:PRO:HB3 | 7:HI:66:VAL:HA | 1.90 | 0.52 |
| 7:HH:231:GLY:HA2 | 7:HI:222:GLU:HG3 | 1.90 | 0.52 |
| 7:HJ:232:THR:HG22 | 7:HJ:235:GLU:HG3 | 1.92 | 0.52 |
| 7:HI:447:HIS:CD2 | 7:HJ:447:HIS:CD2 | 2.97 | 0.52 |
| 9:IC:87:ARG:O | 9:IC:113:ILE:HG12 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:ID:132:SER:OG | 10:ID:135:ASP:HB2 | 2.08 | 0.52 |
| 5:K:54:ALA:HB2 | 5:K:71:ASN:O | 2.09 | 0.52 |
| 7:O:511:GLU:HB3 | 7:O:513:ARG:NH1 | 2.23 | 0.52 |
| 7:P:440:GLN:OE1 | 7:P:511:GLU:HG3 | 2.08 | 0.52 |
| 7:Q:176:ILE:HG23 | 7:Q:177:ALA:H | 1.73 | 0.52 |
| 7:O:407:SER:N | 7:Q:394:ASP:OD2 | 2.36 | 0.52 |
| 8:S:67:ASP:OD1 | 8:S:68:ASP:N | 2.42 | 0.52 |
| 12:W:247:VAL:HG12 | 12:W:248:MET:N | 2.23 | 0.52 |
| 13:YA:148[B]:GLN:OE1 | 13:YA:381[B]:SER:HB2 | 2.09 | 0.52 |
| 13:YA:481[F]:PHE:O | 13:YB:473[F]:GLN:HA | 2.09 | 0.52 |
| 13:YB:256[B]:ILE:HA | 13:YB:286[B]:VAL:HG21 | 1.91 | 0.52 |
| 13:YA:442[B]:THR:HA | 13:YB:434[B]:THR:O | 2.09 | 0.52 |
| 13:YA:442[D]:THR:HA | 13:YB:434[D]:THR:O | 2.09 | 0.52 |
| 13:YB:538[A]:VAL:HG11 | 13:YC:534[A]:LEU:CB | 2.38 | 0.52 |
| 13:YB:26[C]:ARG:HA | 13:YB:55[C]:MET:O | 2.08 | 0.52 |
| 13:YB:18[E]:ARG:HG3 | 13:YC:388[E]:PRO:HG3 | 1.91 | 0.52 |
| 13:YC:16[E]:GLU:OE2 | 13:YC:39[E]:ARG:NH2 | 2.42 | 0.52 |
| 13:YA:495[E]:THR:HA | 13:YC:503[E]:THR:O | 2.08 | 0.52 |
| 13:YC:66[B]:MET:O | 13:YC:69[B]:ILE:N | 2.43 | 0.52 |
| 14:YE:123[E]:PRO:HA | 14:YE:161[E]:PRO:HA | 1.90 | 0.52 |
| 14:YE:330[F]:LYS:HA | 14:YE:330[F]:LYS:HE3 | 1.91 | 0.52 |
| 14:YE:360[D]:ASN:N | 14:YE:360[D]:ASN:HD22 | 1.97 | 0.52 |
| 14:YE:360[D]:ASN:ND2 | 14:YE:360[D]:ASN:H | 2.04 | 0.52 |
| 14:YD:92[F]:HIS:NE2 | 14:YF:238[F]:THR:OG1 | 2.42 | 0.52 |
| 14:YF:330[B]:LYS:HE3 | 14:YF:330[B]:LYS:HA | 1.90 | 0.52 |
| 2:Z:934:ALA:HB1 | 2:Z:942:ILE:HD12 | 1.91 | 0.52 |
| 1:A:299:ASN:OD1 | 1:A:300:ILE:N | 2.42 | 0.52 |
| 4:AA:111:ASN:HD21 | 4:AA:116:ILE:H | 1.56 | 0.52 |
| 4:AA:131:LYS:HD2 | 4:AA:151:ILE:HD13 | 1.91 | 0.52 |
| 5:AD:426:ASP:O | 5:AD:479:LYS:NZ | 2.42 | 0.52 |
| 6:AF:13:ARG:NH1 | 6:AH:17:PHE:O | 2.35 | 0.52 |
| 7:AI:161:THR:OG1 | 7:AI:164:LYS:HE3 | 2.09 | 0.52 |
| 7:AI:511:GLU:HB3 | 7:AI:513:ARG:HH11 | 1.74 | 0.52 |
| 1:B:519:SER:HB3 | 1:B:533:ASP:OD2 | 2.09 | 0.52 |
| 1:B:69:GLN:OE1 | 11:V:70:TYR:HE1 | 1.92 | 0.52 |
| 7:AI:56:GLY:CA | 7:BA:57:ILE:HG23 | 2.39 | 0.52 |
| 1:BH:353:PHE:CD2 | 1:BH:392:ILE:HD13 | 2.44 | 0.52 |
| 1:BH:80:MET:HE3 | 1:BH:326:ARG:HA | 1.90 | 0.52 |
| 2:BJ:494:GLU:HG3 | 2:BJ:498:TRP:CD2 | 2.44 | 0.52 |
| 2:BJ:821:ILE:HG22 | 2:BJ:822:ALA:N | 2.25 | 0.52 |
| 2:C:106:ASN:OD1 | 2:C:107:ALA:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:180:ILE:HA | 2:C:219:TRP:CH2 | 2.45 | 0.52 |
| 2:C:408:HIS:ND1 | 2:C:410:GLU:OE2 | 2.42 | 0.52 |
| 4:CE:27:GLY:HA2 | 4:CE:30:LYS:HD2 | 1.91 | 0.52 |
| 5:CF:144:GLU:N | 5:CF:144:GLU:OE1 | 2.43 | 0.52 |
| 5:CF:206:PHE:CG | 5:CF:223:VAL:HA | 2.44 | 0.52 |
| 2:BJ:221:ALA:N | 5:CG:562:SER:OG | 2.38 | 0.52 |
| 5:CG:569:TYR:HE1 | 5:CH:544:VAL:HG22 | 1.74 | 0.52 |
| 5:CH:272:SER:OG | 6:DA:106:THR:N | 2.27 | 0.52 |
| 6:CI:200:THR:OG1 | 6:CJ:204:ASP:OD2 | 2.26 | 0.52 |
| 3:D:43:ARG:H | 3:D:74:HIS:HB3 | 1.74 | 0.52 |
| 7:DC:20:PRO:HG3 | 7:DC:29:ILE:HG13 | 1.91 | 0.52 |
| 7:DD:289:GLN:OE1 | 7:DD:294:GLN:NE2 | 2.41 | 0.52 |
| 8:DF:36:CYS:HA | 8:DF:73:VAL:HG12 | 1.91 | 0.52 |
| 12:BG:143:TYR:OH | 10:DH:218:ASP:OD2 | 2.21 | 0.52 |
| 11:DI:31:ASN:OD1 | 11:DI:32:TYR:N | 2.41 | 0.52 |
| 3:E:202:ARG:O | 3:E:248:ARG:NH1 | 2.42 | 0.52 |
| 1:EA:174:ARG:NH2 | 1:EA:269:VAL:HG21 | 2.25 | 0.52 |
| 1:EA:18:PRO:O | 1:EA:19:GLU:HG2 | 2.10 | 0.52 |
| 1:EB:555:ILE:O | 1:EB:589:TYR:HD1 | 1.93 | 0.52 |
| 2:EC:193:MET:N | 2:EC:200:TYR:O | 2.37 | 0.52 |
| 1:EA:5:PRO:HG2 | 2:EC:674:TYR:HA | 1.91 | 0.52 |
| 2:EC:703:TYR:OH | 2:EC:725:ARG:NH1 | 2.43 | 0.52 |
| 4:EG:111:ASN:HD21 | 4:EG:116:ILE:H | 1.56 | 0.52 |
| 4:EH:27:GLY:HA2 | 4:EH:30:LYS:HD2 | 1.91 | 0.52 |
| 5:EI:255:ARG:CZ | 5:FA:390:LEU:HD12 | 2.39 | 0.52 |
| 5:EI:468:ASN:OD1 | 5:EI:478:TRP:HB2 | 2.09 | 0.52 |
| 5:EI:64:TRP:CE2 | 5:EI:82:PRO:HG2 | 2.45 | 0.52 |
| 5:EJ:94:ARG:HD3 | 5:EJ:134:GLU:HG2 | 1.89 | 0.52 |
| 5:EJ:180:VAL:HG13 | 5:EJ:181:PHE:H | 1.73 | 0.52 |
| 5:EJ:86:VAL:HG13 | 5:EJ:87:ASN:N | 2.24 | 0.52 |
| 5:FA:319:GLU:OE2 | 5:FA:324:VAL:HG13 | 2.10 | 0.52 |
| 7:FG:34:ALA:HA | 7:FG:37:ALA:HB3 | 1.91 | 0.52 |
| 9:FJ:95:VAL:HG22 | 9:FJ:106:VAL:HG22 | 1.92 | 0.52 |
| 11:GB:30:ARG:HH12 | 11:GB:192:TYR:HD1 | 1.56 | 0.52 |
| 1:GE:448:TYR:CD1 | 1:GE:452:VAL:HG11 | 2.44 | 0.52 |
| 2:GF:408:HIS:ND1 | 2:GF:410:GLU:OE2 | 2.42 | 0.52 |
| 5:HB:49:TRP:CD1 | 5:HB:67:SER:HB3 | 2.44 | 0.52 |
| 5:HB:72:THR:HG22 | 5:HB:77:VAL:HG22 | 1.91 | 0.52 |
| 5:HC:323:THR:CG2 | 5:HC:359:GLU:HB2 | 2.39 | 0.52 |
| 5:HC:426:ASP:O | 5:HC:479:LYS:NZ | 2.42 | 0.52 |
| 5:HC:86:VAL:HG22 | 5:HC:87:ASN:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:98:VAL:CG1 | 5:HC:99:PHE:HD2 | 2.21 | 0.52 |
| 5:HD:206:PHE:CD2 | 5:HD:223:VAL:HA | 2.44 | 0.52 |
| 5:HD:397:ASP:O | 5:HD:400:ILE:HG22 | 2.10 | 0.52 |
| 6:HE:195:LEU:HD13 | 6:HE:215:PHE:HE1 | 1.74 | 0.52 |
| 7:HH:336:GLU:O | 7:HH:340:THR:N | 2.36 | 0.52 |
| 7:HI:472:ARG:HG3 | 7:HI:473:LYS:HG3 | 1.92 | 0.52 |
| 7:HJ:176:ILE:HG23 | 7:HJ:177:ALA:H | 1.73 | 0.52 |
| 7:HJ:77:THR:CG2 | 7:HJ:80:THR:H | 2.23 | 0.52 |
| 5:I:78:THR:HA | 5:I:108:THR:HB | 1.90 | 0.52 |
| 5:I:289:LYS:HE2 | 5:I:370:HIS:HE1 | 1.74 | 0.52 |
| 9:IC:61:LEU:HG | 9:IC:69:THR:HG23 | 1.91 | 0.52 |
| 5:K:107:VAL:O | 5:K:125:GLU:HG3 | 2.09 | 0.52 |
| 5:K:354:THR:HG22 | 5:K:372:ASP:CG | 2.30 | 0.52 |
| 7:P:47:VAL:HG12 | 7:P:48:PRO:N | 2.24 | 0.52 |
| 7:P:518:SER:HB3 | 7:Q:403:SER:HA | 1.90 | 0.52 |
| 7:Q:77:THR:CG2 | 7:Q:80:THR:H | 2.23 | 0.52 |
| 8:R:36:CYS:HA | 8:R:73:VAL:HG12 | 1.91 | 0.52 |
| 8:R:67:ASP:OD1 | 8:R:68:ASP:N | 2.42 | 0.52 |
| 1:X:286:PHE:HB2 | 1:X:300:ILE:CD1 | 2.39 | 0.52 |
| 1:X:522:LYS:HB3 | 1:X:533:ASP:HA | 1.90 | 0.52 |
| 1:Y:209:TRP:HB2 | 1:Y:225:TYR:HE1 | 1.75 | 0.52 |
| 1:Y:103:LYS:N | 1:Y:319:PRO:HB3 | 2.24 | 0.52 |
| 1:Y:400:ASN:ND2 | 1:Y:406:PRO:HD3 | 2.25 | 0.52 |
| 13:YA:148[A]:GLN:OE1 | 13:YA:381[A]:SER:HB2 | 2.09 | 0.52 |
| 13:YA:256[D]:ILE:HA | 13:YA:286[D]:VAL:HG21 | 1.92 | 0.52 |
| 13:YA:76[C]:PRO:C | 13:YA:98[C]:GLY:HA2 | 2.29 | 0.52 |
| 13:YB:256[A]:ILE:HA | 13:YB:286[A]:VAL:HG21 | 1.92 | 0.52 |
| 13:YC:116[B]:ASP:OD2 | 13:YC:121[B]:TYR:N | 2.42 | 0.52 |
| 13:YC:16[D]:GLU:OE2 | 13:YC:39[D]:ARG:NH2 | 2.41 | 0.52 |
| 13:YC:270[A]:ASN:O | 13:YC:274[A]:GLN:N | 2.42 | 0.52 |
| 13:YC:16[F]:GLU:OE2 | 13:YC:39[F]:ARG:NH2 | 2.42 | 0.52 |
| 13:YB:554[D]:MET:HG3 | 13:YC:550[D]:TRP:HB2 | 1.91 | 0.52 |
| 14:YD:123[B]:PRO:HA | 14:YD:161[B]:PRO:HA | 1.90 | 0.52 |
| 14:YD:232[D]:TYR:HD2 | 14:YD:233[D]:ASP:OD1 | 1.92 | 0.52 |
| 14:YD:73[B]:SER:OG | 14:YD:85[B]:THR:OG1 | 2.27 | 0.52 |
| 14:YD:73[D]:SER:OG | 14:YD:85[D]:THR:OG1 | 2.27 | 0.52 |
| 14:YE:232[F]:TYR:HD2 | 14:YE:233[F]:ASP:OD1 | 1.92 | 0.52 |
| 14:YE:238[B]:THR:OG1 | 14:YF:92[B]:HIS:NE2 | 2.42 | 0.52 |
| 14:YF:124[A]:PHE:CE2 | 14:YF:135[A]:MET:HE2 | 2.44 | 0.52 |
| 14:YF:232[A]:TYR:HD2 | 14:YF:233[A]:ASP:OD1 | 1.93 | 0.52 |
| 14:YF:73[A]:SER:OG | 14:YF:85[A]:THR:OG1 | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:174:ARG:NH2 | 1:A:269:VAL:HG21 | 2.25 | 0.52 |
| 1:A:508:ARG:NH2 | 1:A:576:ASP:O | 2.42 | 0.52 |
| 5:AC:486:VAL:HG11 | 5:AE:590:GLN:HE21 | 1.75 | 0.52 |
| 5:AC:67:SER:HB2 | 5:AC:94:ARG:HB2 | 1.91 | 0.52 |
| 5:AD:132:ASP:HB2 | 5:AD:149:LYS:HG3 | 1.91 | 0.52 |
| 5:AE:362:GLU:HB2 | 5:AE:365:ILE:O | 2.09 | 0.52 |
| 5:AE:339:GLU:HG2 | 6:AF:173:THR:HB | 1.90 | 0.52 |
| 6:AG:29:VAL:O | 6:AG:32:ARG:N | 2.36 | 0.52 |
| 1:B:41:ASN:OD1 | 1:B:42:GLU:N | 2.37 | 0.52 |
| 1:B:517:PHE:N | 1:B:536:TYR:O | 2.43 | 0.52 |
| 1:B:67:ILE:HA | 1:B:70:PHE:HB3 | 1.90 | 0.52 |
| 8:BB:50:PRO:HB2 | 8:BB:57:LYS:HD3 | 1.91 | 0.52 |
| 8:BC:115:GLN:HG2 | 8:DF:79:HIS:HE2 | 1.75 | 0.52 |
| 8:BC:5:ASP:OD1 | 8:BC:8:ARG:NH1 | 2.43 | 0.52 |
| 12:BG:125:ILE:HA | 12:BG:162:PHE:CB | 2.39 | 0.52 |
| 1:BH:18:PRO:O | 1:BH:19:GLU:HG2 | 2.10 | 0.52 |
| 1:BI:433:GLU:O | 1:BI:436:LEU:N | 2.42 | 0.52 |
| 2:BJ:326:VAL:HG11 | 2:BJ:413:TRP:CZ2 | 2.44 | 0.52 |
| 2:BJ:969:TYR:O | 2:BJ:973:ASN:N | 2.29 | 0.52 |
| 2:C:299:THR:O | 2:C:349:LEU:HD22 | 2.09 | 0.52 |
| 2:C:234:SER:OG | 2:C:366:TYR:O | 2.25 | 0.52 |
| 5:CF:79:ILE:HG13 | 5:CF:108:THR:O | 2.10 | 0.52 |
| 5:CF:258:TYR:HE1 | 5:CF:384:THR:HG23 | 1.74 | 0.52 |
| 5:CF:289:LYS:HE2 | 5:CF:370:HIS:HE1 | 1.74 | 0.52 |
| 5:CH:79:ILE:HD11 | 5:CH:109:LEU:HG | 1.91 | 0.52 |
| 5:CH:354:THR:HG22 | 5:CH:372:ASP:CG | 2.30 | 0.52 |
| 6:CJ:195:LEU:HD13 | 6:CJ:215:PHE:HE1 | 1.74 | 0.52 |
| 7:DB:146:SER:HB3 | 7:DB:148:PRO:HD2 | 1.91 | 0.52 |
| 7:DB:59:PHE:CZ | 7:DC:55:LYS:HG3 | 2.44 | 0.52 |
| 8:DE:36:CYS:HA | 8:DE:73:VAL:HG12 | 1.91 | 0.52 |
| 8:DF:5:ASP:OD1 | 8:DF:8:ARG:NH1 | 2.43 | 0.52 |
| 11:DI:30:ARG:HH12 | 11:DI:192:TYR:HD1 | 1.56 | 0.52 |
| 11:DI:61:ASN:O | 11:DI:65:GLY:N | 2.38 | 0.52 |
| 1:EA:627:PRO:HG3 | 1:EA:632:ILE:HD11 | 1.92 | 0.52 |
| 2:EC:389:ASN:O | 2:EC:393:SER:OG | 2.21 | 0.52 |
| 2:EC:446:SER:HB2 | 2:EC:485:TYR:OH | 2.09 | 0.52 |
| 3:EE:122:THR:HG22 | 3:EE:169:PRO:HG2 | 1.91 | 0.52 |
| 4:EG:27:GLY:HA2 | 4:EG:30:LYS:HD2 | 1.91 | 0.52 |
| 5:EJ:323:THR:CG2 | 5:EJ:359:GLU:HB2 | 2.39 | 0.52 |
| 5:EJ:44:TYR:CD2 | 5:EJ:48:ALA:HB2 | 2.37 | 0.52 |
| 5:EJ:86:VAL:HG22 | 5:EJ:87:ASN:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:102:TRP:HB2 | 5:FA:129:ARG:O | 2.10 | 0.52 |
| 5:FA:79:ILE:HD11 | 5:FA:109:LEU:HG | 1.91 | 0.52 |
| 5:EI:318:GLN:NE2 | 6:FD:4:LEU:HA | 2.24 | 0.52 |
| 7:FE:118:PRO:HG3 | 7:FF:106:ALA:HA | 1.91 | 0.52 |
| 7:FF:84:ARG:NH1 | 7:FF:88:PRO:HB3 | 2.25 | 0.52 |
| 7:FE:56:GLY:CA | 7:FG:57:ILE:HG23 | 2.39 | 0.52 |
| 1:GD:619:GLN:HG2 | 1:GD:620:THR:HG23 | 1.92 | 0.52 |
| 2:GF:177:GLN:HG3 | 2:GF:215:LYS:HB2 | 1.90 | 0.52 |
| 4:GI:111:ASN:OD1 | 4:GI:114:GLY:N | 2.41 | 0.52 |
| 4:H:131:LYS:HD3 | 4:H:161:ASN:ND2 | 2.25 | 0.52 |
| 4:HA:131:LYS:HD3 | 4:HA:161:ASN:ND2 | 2.25 | 0.52 |
| 5:HB:102:TRP:HB2 | 5:HB:129:ARG:O | 2.10 | 0.52 |
| 5:HB:264:ARG:HA | 5:HB:379:ASP:O | 2.09 | 0.52 |
| 5:HB:469:PRO:HB2 | 5:HB:478:TRP:CD1 | 2.44 | 0.52 |
| 7:HI:84:ARG:NH1 | 7:HI:88:PRO:HB3 | 2.25 | 0.52 |
| 5:I:79:ILE:HG13 | 5:I:108:THR:O | 2.10 | 0.52 |
| 5:I:64:TRP:CE2 | 5:I:82:PRO:HG2 | 2.45 | 0.52 |
| 8:IA:5:ASP:OD1 | 8:IA:8:ARG:NH1 | 2.43 | 0.52 |
| 8:IB:50:PRO:HB2 | 8:IB:57:LYS:HD3 | 1.91 | 0.52 |
| 8:IB:72:THR:HA | 8:IB:154:GLU:HA | 1.92 | 0.52 |
| 12:IF:30:PRO:HG3 | 12:IF:197:ALA:HB2 | 1.92 | 0.52 |
| 2:C:221:ALA:N | 5:J:562:SER:OG | 2.40 | 0.52 |
| 5:K:397:ASP:O | 5:K:400:ILE:HG22 | 2.10 | 0.52 |
| 5:J:569:TYR:OH | 5:K:571:GLU:OE2 | 2.13 | 0.52 |
| 5:K:6:ASN:OD1 | 5:K:17:ASP:HB2 | 2.09 | 0.52 |
| 5:K:79:ILE:HD11 | 5:K:109:LEU:HG | 1.91 | 0.52 |
| 9:T:95:VAL:HG22 | 9:T:106:VAL:HG22 | 1.92 | 0.52 |
| 11:V:45:LEU:HD23 | 11:V:170:LYS:HB3 | 1.91 | 0.52 |
| 12:W:223:VAL:HA | 12:W:241:VAL:HA | 1.92 | 0.52 |
| 1:X:18:PRO:O | 1:X:19:GLU:HG2 | 2.10 | 0.52 |
| 1:X:174:ARG:NH2 | 1:X:269:VAL:HG21 | 2.25 | 0.52 |
| 13:YA:270[F]:ASN:O | 13:YA:274[F]:GLN:N | 2.42 | 0.52 |
| 13:YC:256[E]:ILE:HA | 13:YC:286[E]:VAL:HG21 | 1.91 | 0.52 |
| 13:YA:520[D]:THR:O | 13:YC:529[D]:THR:N | 2.42 | 0.52 |
| 13:YB:538[F]:VAL:HG11 | 13:YC:534[F]:LEU:CB | 2.39 | 0.52 |
| 13:YA:393[B]:MET:HA | 13:YC:71[B]:GLY:HA2 | 1.92 | 0.52 |
| 14:YD:230[F]:LEU:HB2 | 14:YD:313[F]:ILE:HD11 | 1.91 | 0.52 |
| 14:YE:230[F]:LEU:HB2 | 14:YE:313[F]:ILE:HD11 | 1.91 | 0.52 |
| 14:YF:232[C]:TYR:HD2 | 14:YF:233[C]:ASP:OD1 | 1.92 | 0.52 |
| 14:YF:278[F]:SER:O | 14:YF:279[F]:ARG:NH1 | 2.41 | 0.52 |
| 14:YF:230[D]:LEU:HB2 | 14:YF:313[D]:ILE:HD11 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:230[F]:LEU:HB2 | 14:YF:313[F]:ILE:HD11 | 1.91 | 0.52 |
| 14:YF:330[D]:LYS:HE3 | 14:YF:330[D]:LYS:HA | 1.92 | 0.52 |
| 14:YF:360[B]:ASN:H | 14:YF:360[B]:ASN:ND2 | 2.04 | 0.52 |
| 2:Z:138:ASN:OD1 | 2:Z:139:ASN:ND2 | 2.42 | 0.52 |
| 2:Z:258:LYS:HG2 | 2:Z:292:GLU:HG3 | 1.92 | 0.52 |
| 2:Z:299:THR:O | 2:Z:349:LEU:HD22 | 2.09 | 0.52 |
| 15:ZA:16[F]:ALA:HB3 | 15:ZA:48[F]:GLU:HB2 | 1.91 | 0.52 |
| 1:A:560:SER:HA | 1:A:588:LYS:HD3 | 1.92 | 0.52 |
| 4:AA:131:LYS:HD3 | 4:AA:161:ASN:ND2 | 2.25 | 0.52 |
| 5:AC:117:ILE:HG13 | 5:AC:118:LYS:H | 1.73 | 0.52 |
| 5:AC:361:ASP:OD1 | 5:AC:362:GLU:N | 2.43 | 0.52 |
| 5:AC:264:ARG:HA | 5:AC:379:ASP:O | 2.09 | 0.52 |
| 5:AC:468:ASN:OD1 | 5:AC:478:TRP:HB2 | 2.09 | 0.52 |
| 5:AE:354:THR:HG22 | 5:AE:372:ASP:CG | 2.30 | 0.52 |
| 7:BA:457:LEU:HD23 | 7:BA:477:TRP:CZ2 | 2.43 | 0.52 |
| 11:BF:73:LEU:HD22 | 11:BF:86:TRP:HH2 | 1.75 | 0.52 |
| 12:BG:30:PRO:HG3 | 12:BG:197:ALA:HB2 | 1.92 | 0.52 |
| 12:BG:223:VAL:HA | 12:BG:241:VAL:HA | 1.92 | 0.52 |
| 1:BH:238:PHE:HE1 | 1:BH:262:PRO:HD2 | 1.73 | 0.52 |
| 1:BH:400:ASN:O | 1:BI:341:THR:HA | 2.09 | 0.52 |
| 1:BI:555:ILE:O | 1:BI:589:TYR:HD1 | 1.92 | 0.52 |
| 2:BJ:106:ASN:OD1 | 2:BJ:107:ALA:N | 2.43 | 0.52 |
| 2:BJ:12:ARG:HG3 | 2:BJ:24:ARG:HB2 | 1.92 | 0.52 |
| 2:BJ:206:GLN:C | 2:BJ:208:VAL:H | 2.12 | 0.52 |
| 2:BJ:555:ARG:HD3 | 2:BJ:557:VAL:HB | 1.90 | 0.52 |
| 2:BJ:853:ASP:HB2 | 2:BJ:855:ILE:HG22 | 1.92 | 0.52 |
| 2:C:326:VAL:HG11 | 2:C:413:TRP:CZ2 | 2.44 | 0.52 |
| 4:CC:131:LYS:HD2 | 4:CC:151:ILE:HD13 | 1.91 | 0.52 |
| 4:CC:27:GLY:HA2 | 4:CC:30:LYS:HD2 | 1.91 | 0.52 |
| 4:CD:27:GLY:HA2 | 4:CD:30:LYS:HD2 | 1.91 | 0.52 |
| 5:CF:560:ASP:HB3 | 5:CF:561:GLU:OE1 | 2.09 | 0.52 |
| 5:CG:356:TYR:CE1 | 6:CI:4:LEU:HD13 | 2.44 | 0.52 |
| 5:CF:446:VAL:HG21 | 5:CG:443:PHE:CD2 | 2.44 | 0.52 |
| 5:CH:290:SER:HB3 | 5:CH:371:PHE:H | 1.75 | 0.52 |
| 5:CF:552:VAL:HG11 | 5:CH:569:TYR:CE2 | 2.44 | 0.52 |
| 3:D:44:SER:HB3 | 3:D:76:MET:SD | 2.50 | 0.52 |
| 7:DB:110:VAL:HG12 | 7:DB:111:ASN:H | 1.74 | 0.52 |
| 7:DD:232:THR:HG22 | 7:DD:235:GLU:HG3 | 1.92 | 0.52 |
| 7:DC:518:SER:HB3 | 7:DD:403:SER:HA | 1.90 | 0.52 |
| 10:DH:286:VAL:HG22 | 10:DH:287:VAL:H | 1.73 | 0.52 |
| 12:DJ:223:VAL:HA | 12:DJ:241:VAL:HA | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:238:PHE:CE1 | 1:EA:262:PRO:HD2 | 2.44 | 0.52 |
| 1:EB:103:LYS:N | 1:EB:319:PRO:HB3 | 2.24 | 0.52 |
| 1:EB:517:PHE:N | 1:EB:536:TYR:O | 2.43 | 0.52 |
| 2:EC:241:SER:O | 2:EC:244:THR:OG1 | 2.25 | 0.52 |
| 1:EB:402:ALA:HB2 | 2:EC:741:GLU:HA | 1.92 | 0.52 |
| 3:EE:202:ARG:O | 3:EE:248:ARG:NH1 | 2.42 | 0.52 |
| 5:EI:92:VAL:HG12 | 5:EI:136:VAL:HG12 | 1.91 | 0.52 |
| 5:EI:206:PHE:CG | 5:EI:223:VAL:HA | 2.44 | 0.52 |
| 5:EI:486:VAL:HG11 | 5:FA:590:GLN:HE21 | 1.75 | 0.52 |
| 5:EI:20:ARG:CZ | 5:FA:7:ILE:HD12 | 2.40 | 0.52 |
| 7:FE:161:THR:OG1 | 7:FE:164:LYS:HE3 | 2.09 | 0.52 |
| 7:FE:383:TYR:CD1 | 7:FE:393:PRO:HG3 | 2.44 | 0.52 |
| 7:FE:49:ASP:O | 7:FE:56:GLY:HA3 | 2.09 | 0.52 |
| 7:FF:515:TRP:CZ2 | 7:FG:439:ILE:HG23 | 2.44 | 0.52 |
| 8:FH:67:ASP:OD1 | 8:FH:68:ASP:N | 2.42 | 0.52 |
| 2:GF:782:VAL:HA | 2:GF:795:VAL:HG23 | 1.92 | 0.52 |
| 2:GF:900:ILE:HG13 | 3:GH:311:TYR:CE1 | 2.44 | 0.52 |
| 4:HA:124:ILE:HD12 | 4:HA:137:LEU:HD23 | 1.90 | 0.52 |
| 5:HB:468:ASN:OD1 | 5:HB:478:TRP:HB2 | 2.09 | 0.52 |
| 5:HB:486:VAL:HG11 | 5:HD:590:GLN:HE21 | 1.74 | 0.52 |
| 5:HC:249:ASP:CA | 5:HD:158:ASP:HB3 | 2.39 | 0.52 |
| 5:HD:6:ASN:OD1 | 5:HD:17:ASP:HB2 | 2.09 | 0.52 |
| 6:HF:195:LEU:HD13 | 6:HF:215:PHE:HE1 | 1.74 | 0.52 |
| 7:HH:451:PHE:HD1 | 7:HH:469:VAL:HG13 | 1.75 | 0.52 |
| 7:HI:210:ILE:O | 7:HJ:210:ILE:HG22 | 2.10 | 0.52 |
| 7:HI:20:PRO:HG3 | 7:HI:29:ILE:HG13 | 1.91 | 0.52 |
| 7:HI:341:ILE:HG13 | 7:HJ:341:ILE:HD11 | 1.90 | 0.52 |
| 7:HJ:255:SER:HB3 | 7:HJ:263:VAL:CG1 | 2.40 | 0.52 |
| 5:I:20:ARG:CZ | 5:K:7:ILE:HD12 | 2.40 | 0.52 |
| 9:IC:125:GLN:N | 9:IC:125:GLN:OE1 | 2.43 | 0.52 |
| 12:GC:251:GLY:HA3 | 12:IF:104:PHE:CG | 2.45 | 0.52 |
| 5:K:261:ARG:HD2 | 5:K:297:GLY:HA3 | 1.92 | 0.52 |
| 5:J:569:TYR:HE1 | 5:K:544:VAL:HG22 | 1.74 | 0.52 |
| 6:L:54:SER:O | 6:M:164:GLN:NE2 | 2.42 | 0.52 |
| 6:N:195:LEU:HD13 | 6:N:215:PHE:HE1 | 1.74 | 0.52 |
| 7:O:161:THR:OG1 | 7:O:164:LYS:HE3 | 2.09 | 0.52 |
| 7:P:399:PHE:HZ | 7:P:516:ASN:HD22 | 1.58 | 0.52 |
| 7:P:406:GLY:O | 7:P:410:THR:HG23 | 2.10 | 0.52 |
| 7:P:472:ARG:HG3 | 7:P:473:LYS:HG3 | 1.92 | 0.52 |
| 7:P:210:ILE:O | 7:Q:210:ILE:HG22 | 2.09 | 0.52 |
| 8:S:72:THR:HA | 8:S:154:GLU:HA | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:U:323:LYS:HB3 | 10:U:339:PRO:HG3 | 1.92 | 0.52 |
| 1:X:299:ASN:OD1 | 1:X:300:ILE:N | 2.42 | 0.52 |
| 13:YA:116[E]:ASP:OD2 | 13:YA:121[E]:TYR:N | 2.42 | 0.52 |
| 13:YA:270[B]:ASN:O | 13:YA:274[B]:GLN:N | 2.42 | 0.52 |
| 13:YA:379[C]:PRO:HG2 | 13:YA:429[C]:ARG:CZ | 2.40 | 0.52 |
| 13:YA:16[B]:GLU:OE2 | 13:YA:39[B]:ARG:NH2 | 2.42 | 0.52 |
| 13:YA:61[B]:ILE:HG21 | 13:YB:59[B]:GLN:HA | 1.92 | 0.52 |
| 13:YA:9[E]:ASN:HA | 13:YC:7[E]:ASN:ND2 | 2.17 | 0.52 |
| 13:YB:256[E]:ILE:HA | 13:YB:286[E]:VAL:HG21 | 1.91 | 0.52 |
| 13:YB:270[D]:ASN:O | 13:YB:274[D]:GLN:N | 2.42 | 0.52 |
| 13:YB:256[D]:ILE:HA | 13:YB:286[D]:VAL:HG21 | 1.92 | 0.52 |
| 13:YA:442[F]:THR:HA | 13:YB:434[F]:THR:O | 2.09 | 0.52 |
| 13:YA:454[D]:LYS:NZ | 13:YB:464[D]:TYR:OH | 2.42 | 0.52 |
| 13:YB:527[F]:THR:O | 13:YC:519[F]:THR:HA | 2.08 | 0.52 |
| 13:YA:76[D]:PRO:HA | 13:YC:61[D]:ILE:HA | 1.90 | 0.52 |
| 14:YD:230[E]:LEU:HB2 | 14:YD:313[E]:ILE:HD11 | 1.91 | 0.52 |
| 14:YD:232[B]:TYR:HD2 | 14:YD:233[B]:ASP:OD1 | 1.92 | 0.52 |
| 14:YD:230[B]:LEU:HB2 | 14:YD:313[B]:ILE:HD11 | 1.91 | 0.52 |
| 14:YD:360[F]:ASN:N | 14:YD:360[F]:ASN:HD22 | 1.98 | 0.52 |
| 14:YD:73[C]:SER:OG | 14:YD:85[C]:THR:OG1 | 2.27 | 0.52 |
| 14:YE:232[E]:TYR:HD2 | 14:YE:233[E]:ASP:OD1 | 1.92 | 0.52 |
| 14:YE:278[A]:SER:O | 14:YE:279[A]:ARG:NH1 | 2.41 | 0.52 |
| 14:YF:330[A]:LYS:HA | 14:YF:330[A]:LYS:HE3 | 1.91 | 0.52 |
| 14:YF:360[C]:ASN:ND2 | 14:YF:360[C]:ASN:H | 2.04 | 0.52 |
| 14:YF:360[B]:ASN:HD22 | 14:YF:360[B]:ASN:N | 1.98 | 0.52 |
| 14:YF:73[F]:SER:OG | 14:YF:85[F]:THR:OG1 | 2.27 | 0.52 |
| 2:Z:106:ASN:OD1 | 2:Z:107:ALA:N | 2.43 | 0.52 |
| 2:Z:450:PHE:HZ | 2:Z:473:TYR:HE1 | 1.56 | 0.52 |
| 1:X:60:LEU:HD22 | 2:Z:671:TYR:CD1 | 2.45 | 0.52 |
| 1:A:130:ARG:HD3 | 14:YD:181[A]:GLY:HA2 | 1.91 | 0.52 |
| 4:AB:111:ASN:HD21 | 4:AB:116:ILE:H | 1.56 | 0.52 |
| 5:AC:257:SER:OG | 5:AC:387:ASN:HB2 | 2.10 | 0.52 |
| 5:AD:291:ILE:HG22 | 5:AD:292:PRO:O | 2.10 | 0.52 |
| 5:AE:78:THR:HA | 5:AE:108:THR:HB | 1.92 | 0.52 |
| 5:AE:206:PHE:CD2 | 5:AE:223:VAL:HA | 2.44 | 0.52 |
| 6:AF:14:LEU:O | 6:AF:16:ASP:N | 2.43 | 0.52 |
| 6:AF:82:VAL:HB | 6:AF:187:LYS:HB3 | 1.92 | 0.52 |
| 6:AG:195:LEU:HD13 | 6:AG:215:PHE:HE1 | 1.74 | 0.52 |
| 1:B:402:ALA:HB2 | 2:C:741:GLU:HA | 1.92 | 0.52 |
| 1:B:433:GLU:O | 1:B:436:LEU:N | 2.42 | 0.52 |
| 8:BC:50:PRO:HB2 | 8:BC:57:LYS:HD3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:BG:23:SER:N | 12:BG:202:ASN:O | 2.29 | 0.52 |
| 12:BG:211:HIS:HE1 | 12:DJ:167:GLU:HA | 1.75 | 0.52 |
| 1:BI:52:ARG:HD3 | 2:BJ:657:TYR:HD1 | 1.74 | 0.52 |
| 1:BI:67:ILE:HA | 1:BI:70:PHE:HB3 | 1.90 | 0.52 |
| 2:BJ:405:VAL:N | 2:BJ:414:LYS:O | 2.41 | 0.52 |
| 2:BJ:450:PHE:HZ | 2:BJ:473:TYR:HE1 | 1.56 | 0.52 |
| 2:C:12:ARG:HG3 | 2:C:24:ARG:HB2 | 1.92 | 0.52 |
| 2:C:821:ILE:HG22 | 2:C:822:ALA:N | 2.25 | 0.52 |
| 5:CF:102:TRP:HB2 | 5:CF:129:ARG:O | 2.10 | 0.52 |
| 5:CF:289:LYS:O | 5:CF:290:SER:OG | 2.24 | 0.52 |
| 5:CF:391:GLY:O | 5:CF:392:THR:OG1 | 2.23 | 0.52 |
| 5:CF:468:ASN:OD1 | 5:CF:478:TRP:HB2 | 2.09 | 0.52 |
| 5:CG:137:TYR:HA | 5:CG:143:TRP:HD1 | 1.72 | 0.52 |
| 5:CG:291:ILE:HG22 | 5:CG:292:PRO:O | 2.10 | 0.52 |
| 6:CI:14:LEU:O | 6:CI:16:ASP:N | 2.43 | 0.52 |
| 7:DC:466:SER:HB3 | 7:DC:468:PHE:CE2 | 2.45 | 0.52 |
| 10:DH:132:SER:OG | 10:DH:135:ASP:HB2 | 2.08 | 0.52 |
| 12:DJ:30:PRO:HG3 | 12:DJ:197:ALA:HB2 | 1.92 | 0.52 |
| 1:EA:508:ARG:NH2 | 1:EA:576:ASP:O | 2.42 | 0.52 |
| 1:EB:156:ASP:HB3 | 1:EB:160:GLN:O | 2.10 | 0.52 |
| 3:ED:43:ARG:H | 3:ED:74:HIS:HB3 | 1.74 | 0.52 |
| 4:EF:201:LYS:HB3 | 4:EF:280:ALA:HB3 | 1.90 | 0.52 |
| 4:EG:53:GLY:HA3 | 4:EH:7:LYS:HE2 | 1.91 | 0.52 |
| 5:EI:118:LYS:NZ | 5:EI:145:TYR:O | 2.37 | 0.52 |
| 5:EI:1:MET:N | 5:EJ:41:ASP:HB3 | 2.25 | 0.52 |
| 5:EI:557:TYR:OH | 5:EJ:556:GLN:OE1 | 2.28 | 0.52 |
| 5:FA:54:ALA:HB2 | 5:FA:71:ASN:O | 2.09 | 0.52 |
| 6:FB:100:PRO:O | 6:FB:103:SER:OG | 2.18 | 0.52 |
| 6:FD:195:LEU:HD13 | 6:FD:215:PHE:HE1 | 1.74 | 0.52 |
| 7:FF:295:ILE:HG12 | 7:FG:301:ARG:HD3 | 1.91 | 0.52 |
| 7:FG:232:THR:HG22 | 7:FG:235:GLU:HG3 | 1.92 | 0.52 |
| 9:FJ:87:ARG:O | 9:FJ:113:ILE:HG12 | 2.09 | 0.52 |
| 1:EB:69:GLN:OE1 | 11:GB:70:TYR:HE1 | 1.92 | 0.52 |
| 1:GD:145:PHE:CD2 | 1:GD:169:GLN:OE1 | 2.63 | 0.52 |
| 1:GD:238:PHE:CE1 | 1:GD:262:PRO:HD2 | 2.44 | 0.52 |
| 2:GF:389:ASN:O | 2:GF:393:SER:OG | 2.21 | 0.52 |
| 1:GD:5:PRO:HG2 | 2:GF:674:TYR:HA | 1.92 | 0.52 |
| 2:GF:91:GLN:NE2 | 2:GF:92:SER:H | 2.06 | 0.52 |
| 3:GG:43:ARG:H | 3:GG:74:HIS:HB3 | 1.73 | 0.52 |
| 4:H:131:LYS:HD2 | 4:H:151:ILE:HD13 | 1.91 | 0.52 |
| 4:HA:131:LYS:HD2 | 4:HA:151:ILE:HD13 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HE:14:LEU:O | 6:HE:16:ASP:N | 2.43 | 0.52 |
| 7:HI:399:PHE:HZ | 7:HI:516:ASN:HD22 | 1.58 | 0.52 |
| 7:HI:466:SER:HB3 | 7:HI:468:PHE:CE2 | 2.45 | 0.52 |
| 5:I:102:TRP:HB2 | 5:I:129:ARG:O | 2.10 | 0.52 |
| 5:I:144:GLU:OE1 | 5:I:144:GLU:N | 2.43 | 0.52 |
| 9:IC:95:VAL:HG22 | 9:IC:106:VAL:HG22 | 1.92 | 0.52 |
| 12:IF:247:VAL:HG12 | 12:IF:248:MET:N | 2.23 | 0.52 |
| 5:J:291:ILE:HG22 | 5:J:292:PRO:O | 2.10 | 0.52 |
| 5:K:127:ASN:HD21 | 5:K:182:ARG:HH12 | 1.56 | 0.52 |
| 6:N:14:LEU:O | 6:N:16:ASP:N | 2.43 | 0.52 |
| 7:O:27:PRO:HA | 7:O:29:ILE:HD11 | 1.92 | 0.52 |
| 7:O:480:ARG:HD3 | 7:P:462:ASN:ND2 | 2.25 | 0.52 |
| 7:O:512:THR:O | 7:Q:514:PRO:HB3 | 2.09 | 0.52 |
| 1:X:80:MET:HE3 | 1:X:326:ARG:HA | 1.92 | 0.52 |
| 13:YA:66[F]:MET:O | 13:YA:69[F]:ILE:N | 2.43 | 0.52 |
| 13:YB:256[C]:ILE:HA | 13:YB:286[C]:VAL:HG21 | 1.92 | 0.52 |
| 13:YB:270[A]:ASN:O | 13:YB:274[A]:GLN:N | 2.42 | 0.52 |
| 13:YB:256[F]:ILE:HA | 13:YB:286[F]:VAL:HG21 | 1.92 | 0.52 |
| 13:YB:460[B]:GLY:N | 13:YC:452[B]:GLY:O | 2.42 | 0.52 |
| 13:YA:481[D]:PHE:O | 13:YB:473[D]:GLN:HA | 2.09 | 0.52 |
| 13:YB:76[C]:PRO:C | 13:YB:98[C]:GLY:HA2 | 2.29 | 0.52 |
| 13:YC:16[C]:GLU:OE2 | 13:YC:39[C]:ARG:NH2 | 2.42 | 0.52 |
| 13:YC:270[B]:ASN:O | 13:YC:274[B]:GLN:N | 2.42 | 0.52 |
| 13:YC:379[C]:PRO:HG2 | 13:YC:429[C]:ARG:CZ | 2.40 | 0.52 |
| 13:YA:520[B]:THR:O | 13:YC:529[B]:THR:N | 2.42 | 0.52 |
| 13:YB:554[E]:MET:HG3 | 13:YC:550[E]:TRP:HB2 | 1.91 | 0.52 |
| 13:YC:18[C]:ARG:NH1 | 13:YC:77[C]:VAL:HG23 | 2.23 | 0.52 |
| 14:YD:124[A]:PHE:CE2 | 14:YD:135[A]:MET:HE2 | 2.44 | 0.52 |
| 14:YD:360[F]:ASN:ND2 | 14:YD:360[F]:ASN:H | 2.04 | 0.52 |
| 14:YD:332[E]:GLN:OE1 | 14:YE:101[E]:GLY:HA2 | 2.10 | 0.52 |
| 14:YE:360[E]:ASN:HD22 | 14:YE:360[E]:ASN:N | 1.98 | 0.52 |
| 14:YE:360[E]:ASN:ND2 | 14:YE:360[E]:ASN:H | 2.04 | 0.52 |
| 14:YF:123[D]:PRO:HA | 14:YF:161[D]:PRO:HA | 1.91 | 0.52 |
| 14:YF:123[C]:PRO:HA | 14:YF:161[C]:PRO:HA | 1.91 | 0.52 |
| 14:YF:230[A]:LEU:HB2 | 14:YF:313[A]:ILE:HD11 | 1.91 | 0.52 |
| 14:YF:232[F]:TYR:HD2 | 14:YF:233[F]:ASP:OD1 | 1.92 | 0.52 |
| 14:YD:97[A]:VAL:HG21 | 14:YF:332[A]:GLN:NE2 | 2.25 | 0.52 |
| 14:YF:360[C]:ASN:HD22 | 14:YF:360[C]:ASN:N | 1.97 | 0.52 |
| 2:Z:935:LYS:HZ2 | 2:Z:936:LEU:HD13 | 1.72 | 0.52 |
| 5:AD:261:ARG:NE | 5:AD:297:GLY:O | 2.30 | 0.52 |
| 7:AJ:472:ARG:HG3 | 7:AJ:473:LYS:HG3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:BB:130:LYS:NZ | 8:BB:163:GLU:OE2 | 2.37 | 0.52 |
| 11:BF:45:LEU:HD23 | 11:BF:170:LYS:HB3 | 1.91 | 0.52 |
| 12:BG:204:HIS:CB | 12:BG:210:PRO:HA | 2.40 | 0.52 |
| 1:BI:209:TRP:HB2 | 1:BI:225:TYR:HE1 | 1.74 | 0.52 |
| 1:BI:363:PHE:CE1 | 1:BI:373:PHE:HD2 | 2.28 | 0.52 |
| 2:C:138:ASN:OD1 | 2:C:139:ASN:ND2 | 2.42 | 0.52 |
| 2:C:258:LYS:HG2 | 2:C:292:GLU:HG3 | 1.92 | 0.52 |
| 2:C:389:ASN:O | 2:C:393:SER:OG | 2.20 | 0.52 |
| 3:CA:226:GLU:OE1 | 3:CA:226:GLU:N | 2.34 | 0.52 |
| 3:CA:31:GLY:O | 3:CA:291:LYS:NZ | 2.31 | 0.52 |
| 3:CB:232:GLN:O | 3:CB:232:GLN:HG2 | 2.10 | 0.52 |
| 5:CG:410:GLN:HG2 | 5:CG:443:PHE:O | 2.10 | 0.52 |
| 5:CH:36:GLU:HA | 5:CH:50:LYS:HZ1 | 1.75 | 0.52 |
| 5:CH:6:ASN:OD1 | 5:CH:17:ASP:HB2 | 2.09 | 0.52 |
| 7:DB:146:SER:O | 7:DB:150:ALA:N | 2.38 | 0.52 |
| 7:DC:406:GLY:O | 7:DC:410:THR:HG23 | 2.10 | 0.52 |
| 8:DF:14:ASP:OD2 | 8:DF:17:ARG:NH2 | 2.33 | 0.52 |
| 8:DF:55:ASN:HB3 | 8:IB:99:ILE:HD11 | 1.91 | 0.52 |
| 12:DJ:126:TYR:CD2 | 12:DJ:163:ARG:HG3 | 2.44 | 0.52 |
| 12:DJ:216:PHE:HE1 | 12:DJ:218:MET:CE | 2.23 | 0.52 |
| 3:E:232:GLN:O | 3:E:232:GLN:HG2 | 2.10 | 0.52 |
| 1:EB:112:LEU:HB3 | 1:EB:300:ILE:HG22 | 1.92 | 0.52 |
| 1:EB:348:PHE:CZ | 1:EB:399:TYR:HD2 | 2.28 | 0.52 |
| 1:EB:433:GLU:O | 1:EB:436:LEU:N | 2.42 | 0.52 |
| 1:EB:538:VAL:HG11 | 1:EB:558:PHE:CE1 | 2.45 | 0.52 |
| 2:EC:183:VAL:HA | 2:EC:210:LYS:HE3 | 1.90 | 0.52 |
| 2:EC:207:PRO:HA | 2:EC:229:VAL:HG23 | 1.90 | 0.52 |
| 2:EC:494:GLU:HG3 | 2:EC:498:TRP:CD2 | 2.44 | 0.52 |
| 4:EF:27:GLY:HA2 | 4:EF:30:LYS:HD2 | 1.91 | 0.52 |
| 4:EF:79:VAL:N | 4:EF:97:ILE:O | 2.32 | 0.52 |
| 5:EI:144:GLU:OE1 | 5:EI:144:GLU:N | 2.43 | 0.52 |
| 5:EI:172:GLN:HG2 | 5:EI:173:GLY:H | 1.75 | 0.52 |
| 5:EI:264:ARG:HA | 5:EI:379:ASP:O | 2.09 | 0.52 |
| 5:EI:552:VAL:HG11 | 5:FA:569:TYR:CE2 | 2.44 | 0.52 |
| 4:F:131:LYS:HD2 | 4:F:151:ILE:HD13 | 1.91 | 0.52 |
| 5:EJ:591:PRO:HA | 5:FA:520:GLY:O | 2.09 | 0.52 |
| 6:FB:29:VAL:O | 6:FB:32:ARG:N | 2.36 | 0.52 |
| 7:FE:110:VAL:HG12 | 7:FE:111:ASN:H | 1.74 | 0.52 |
| 7:FF:325:TYR:CD1 | 7:FF:330:ARG:HA | 2.41 | 0.52 |
| 7:FF:466:SER:HB3 | 7:FF:468:PHE:CE2 | 2.45 | 0.52 |
| 1:GD:444:ILE:O | 1:GD:447:TYR:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GE:209:TRP:HB2 | 1:GE:225:TYR:HE1 | 1.74 | 0.52 |
| 1:GE:547:SER:O | 1:GE:548:LYS:HG2 | 2.10 | 0.52 |
| 2:GF:106:ASN:OD1 | 2:GF:107:ALA:N | 2.43 | 0.52 |
| 2:GF:206:GLN:C | 2:GF:208:VAL:H | 2.12 | 0.52 |
| 2:GF:299:THR:O | 2:GF:349:LEU:HD22 | 2.09 | 0.52 |
| 2:GF:969:TYR:HD2 | 2:GF:982:LEU:HD13 | 1.75 | 0.52 |
| 2:GF:981:GLN:CG | 2:GF:982:LEU:H | 2.19 | 0.52 |
| 5:HB:144:GLU:OE1 | 5:HB:144:GLU:N | 2.43 | 0.52 |
| 5:HB:257:SER:OG | 5:HB:387:ASN:HB2 | 2.09 | 0.52 |
| 5:HB:64:TRP:O | 5:HB:93:ILE:HG22 | 2.10 | 0.52 |
| 5:HC:465:ASN:ND2 | 5:HD:418:GLY:O | 2.42 | 0.52 |
| 6:HG:14:LEU:O | 6:HG:16:ASP:N | 2.43 | 0.52 |
| 6:HG:195:LEU:HD13 | 6:HG:215:PHE:HE1 | 1.74 | 0.52 |
| 7:HH:383:TYR:CD1 | 7:HH:393:PRO:HG3 | 2.44 | 0.52 |
| 7:HI:160:MET:CE | 7:HI:165:THR:HB | 2.40 | 0.52 |
| 7:HH:45:ASN:CG | 7:HI:24:ASN:HD21 | 2.13 | 0.52 |
| 5:I:100:ALA:HB2 | 5:I:130:PHE:CD1 | 2.45 | 0.52 |
| 5:I:94:ARG:CD | 5:I:134:GLU:HG2 | 2.38 | 0.52 |
| 8:IA:50:PRO:HB2 | 8:IA:57:LYS:HD3 | 1.91 | 0.52 |
| 5:J:191:ILE:H | 5:K:164:ARG:HH21 | 1.58 | 0.52 |
| 5:J:86:VAL:HG22 | 5:J:87:ASN:H | 1.75 | 0.52 |
| 5:K:319:GLU:OE2 | 5:K:324:VAL:HG13 | 2.10 | 0.52 |
| 6:M:14:LEU:O | 6:M:16:ASP:N | 2.43 | 0.52 |
| 7:P:146:SER:HA | 7:P:164:LYS:HZ2 | 1.74 | 0.52 |
| 7:P:160:MET:CE | 7:P:165:THR:HB | 2.40 | 0.52 |
| 7:O:449:GLY:N | 7:Q:482:TYR:O | 2.33 | 0.52 |
| 7:P:429:CYS:HG | 7:Q:515:TRP:HE1 | 1.55 | 0.52 |
| 1:X:145:PHE:CD2 | 1:X:169:GLN:OE1 | 2.63 | 0.52 |
| 13:YA:179[E]:MET:SD | 13:YA:279[E]:ASN:ND2 | 2.76 | 0.52 |
| 13:YA:256[A]:ILE:HA | 13:YA:286[A]:VAL:HG21 | 1.92 | 0.52 |
| 13:YA:461[B]:SER:OG | 13:YC:468[B]:ASP:OD2 | 2.27 | 0.52 |
| 13:YA:565[F]:TYR:CE2 | 13:YC:567[F]:ILE:HG23 | 2.44 | 0.52 |
| 13:YA:61[F]:ILE:HA | 13:YB:76[F]:PRO:O | 2.10 | 0.52 |
| 13:YB:71[F]:GLY:HA2 | 13:YC:393[F]:MET:HA | 1.92 | 0.52 |
| 13:YC:256[F]:ILE:HA | 13:YC:286[F]:VAL:HG21 | 1.92 | 0.52 |
| 13:YC:270[D]:ASN:O | 13:YC:274[D]:GLN:N | 2.42 | 0.52 |
| 13:YC:256[B]:ILE:HA | 13:YC:286[B]:VAL:HG21 | 1.91 | 0.52 |
| 13:YB:554[B]:MET:HG3 | 13:YC:550[B]:TRP:HB2 | 1.91 | 0.52 |
| 13:YA:393[F]:MET:HA | 13:YC:71[F]:GLY:HA2 | 1.91 | 0.52 |
| 14:YD:230[D]:LEU:HB2 | 14:YD:313[D]:ILE:HD11 | 1.91 | 0.52 |
| 14:YD:330[A]:LYS:HA | 14:YD:330[A]:LYS:HE3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:124[C]:PHE:CE2 | 14:YE:135[C]:MET:HE2 | 2.45 | 0.52 |
| 10:U:285:LEU:HA | 14:YE:215[E]:GLU:CG | 2.38 | 0.52 |
| 14:YE:232[B]:TYR:HD2 | 14:YE:233[B]:ASP:OD1 | 1.92 | 0.52 |
| 14:YE:230[C]:LEU:HB2 | 14:YE:313[C]:ILE:HD11 | 1.91 | 0.52 |
| 14:YE:73[A]:SER:OG | 14:YE:85[A]:THR:OG1 | 2.27 | 0.52 |
| 14:YF:230[B]:LEU:HB2 | 14:YF:313[B]:ILE:HD11 | 1.91 | 0.52 |
| 14:YD:101[B]:GLY:HA2 | 14:YF:332[B]:GLN:OE1 | 2.09 | 0.52 |
| 2:Z:339:ASP:HB3 | 2:Z:340:PRO:CD | 2.36 | 0.52 |
| 2:Z:703:TYR:OH | 2:Z:725:ARG:NH1 | 2.43 | 0.52 |
| 2:Z:782:VAL:HA | 2:Z:795:VAL:HG23 | 1.92 | 0.52 |
| 4:AB:124:ILE:HD12 | 4:AB:137:LEU:HD23 | 1.90 | 0.52 |
| 5:AC:289:LYS:O | 5:AC:290:SER:OG | 2.24 | 0.52 |
| 5:AC:469:PRO:HB2 | 5:AC:478:TRP:CD1 | 2.44 | 0.52 |
| 5:AD:186:TYR:OH | 5:AD:191:ILE:HA | 2.09 | 0.52 |
| 7:AJ:84:ARG:NH1 | 7:AJ:88:PRO:HB3 | 2.25 | 0.52 |
| 7:BA:167:GLN:O | 7:BA:171:LYS:HG2 | 2.10 | 0.52 |
| 7:BA:375:TYR:CE2 | 7:BA:390:PRO:HB2 | 2.45 | 0.52 |
| 1:BH:282:GLY:N | 1:BH:312:GLY:O | 2.39 | 0.52 |
| 1:BI:156:ASP:HB3 | 1:BI:160:GLN:O | 2.10 | 0.52 |
| 2:BJ:446:SER:HB2 | 2:BJ:485:TYR:OH | 2.09 | 0.52 |
| 2:BJ:39:ALA:HB2 | 2:BJ:56:TRP:CZ3 | 2.44 | 0.52 |
| 2:BJ:572:ASN:HB3 | 2:BJ:611:ILE:HG22 | 1.92 | 0.52 |
| 2:BJ:986:ARG:HH22 | 3:CA:323:ASP:CB | 2.23 | 0.52 |
| 2:C:206:GLN:C | 2:C:208:VAL:H | 2.12 | 0.52 |
| 3:CB:122:THR:HG22 | 3:CB:169:PRO:HG2 | 1.91 | 0.52 |
| 4:CC:124:ILE:HD12 | 4:CC:137:LEU:HD23 | 1.90 | 0.52 |
| 4:CD:79:VAL:N | 4:CD:97:ILE:O | 2.32 | 0.52 |
| 5:CF:361:ASP:OD1 | 5:CF:362:GLU:N | 2.43 | 0.52 |
| 5:CF:257:SER:OG | 5:CF:387:ASN:HB2 | 2.09 | 0.52 |
| 5:CF:51:THR:HA | 5:CF:69:ALA:HB3 | 1.92 | 0.52 |
| 5:CG:400:ILE:O | 5:CG:403:THR:OG1 | 2.27 | 0.52 |
| 5:CH:206:PHE:CD2 | 5:CH:223:VAL:HA | 2.44 | 0.52 |
| 7:DB:100:TYR:CZ | 7:DC:113:GLU:HA | 2.45 | 0.52 |
| 7:DD:173:ILE:O | 7:DD:178:PRO:HD2 | 2.09 | 0.52 |
| 11:DI:45:LEU:HD23 | 11:DI:170:LYS:HB3 | 1.91 | 0.52 |
| 3:E:102:ASP:HB3 | 3:E:105:THR:HB | 1.92 | 0.52 |
| 2:C:9:THR:HG21 | 3:E:57:ALA:HB3 | 1.91 | 0.52 |
| 1:EA:560:SER:HA | 1:EA:588:LYS:HD3 | 1.92 | 0.52 |
| 1:EB:363:PHE:CE1 | 1:EB:373:PHE:HD2 | 2.28 | 0.52 |
| 2:EC:326:VAL:HG11 | 2:EC:413:TRP:CZ2 | 2.44 | 0.52 |
| 3:EE:137:PRO:HG3 | 3:EE:185:GLY:HA3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:100:ALA:HB2 | 5:EI:130:PHE:CD1 | 2.45 | 0.52 |
| 5:EI:560:ASP:HB3 | 5:EI:561:GLU:OE1 | 2.09 | 0.52 |
| 5:EJ:258:TYR:O | 5:EJ:259:THR:OG1 | 2.25 | 0.52 |
| 4:F:131:LYS:HD3 | 4:F:161:ASN:ND2 | 2.25 | 0.52 |
| 5:FA:204:ASP:OD1 | 5:FA:205:VAL:N | 2.43 | 0.52 |
| 5:FA:261:ARG:HD2 | 5:FA:297:GLY:HA3 | 1.92 | 0.52 |
| 7:FF:399:PHE:HZ | 7:FF:516:ASN:HD22 | 1.58 | 0.52 |
| 7:FG:173:ILE:O | 7:FG:178:PRO:HD2 | 2.09 | 0.52 |
| 8:FH:72:THR:HA | 8:FH:154:GLU:HA | 1.92 | 0.52 |
| 4:G:131:LYS:HD2 | 4:G:151:ILE:HD13 | 1.91 | 0.52 |
| 1:GD:627:PRO:HG3 | 1:GD:632:ILE:HD11 | 1.92 | 0.52 |
| 1:GE:192:ILE:HG22 | 1:GE:272:TYR:CD1 | 2.45 | 0.52 |
| 1:GE:555:ILE:O | 1:GE:589:TYR:HD1 | 1.93 | 0.52 |
| 2:GF:107:ALA:HB2 | 2:GF:128:THR:HA | 1.91 | 0.52 |
| 2:GF:234:SER:OG | 2:GF:366:TYR:O | 2.25 | 0.52 |
| 2:GF:703:TYR:OH | 2:GF:725:ARG:NH1 | 2.43 | 0.52 |
| 3:GG:104:TYR:HE2 | 3:GG:165:ARG:NH2 | 2.08 | 0.52 |
| 4:H:27:GLY:HA2 | 4:H:30:LYS:HD2 | 1.91 | 0.52 |
| 5:HB:194:LYS:HB2 | 5:HB:243:GLN:HB2 | 1.92 | 0.52 |
| 5:HB:208:GLU:OE1 | 5:HB:233:ARG:NH2 | 2.43 | 0.52 |
| 5:HD:362:GLU:HB2 | 5:HD:365:ILE:O | 2.09 | 0.52 |
| 5:HD:79:ILE:HD11 | 5:HD:109:LEU:HG | 1.91 | 0.52 |
| 7:HH:146:SER:HB3 | 7:HH:148:PRO:HD2 | 1.91 | 0.52 |
| 7:HH:315:ILE:HG12 | 7:HJ:308:ILE:HD12 | 1.92 | 0.52 |
| 8:IA:72:THR:HA | 8:IA:154:GLU:HA | 1.92 | 0.52 |
| 11:IE:45:LEU:HD23 | 11:IE:170:LYS:HB3 | 1.91 | 0.52 |
| 12:IF:23:SER:N | 12:IF:202:ASN:O | 2.29 | 0.52 |
| 12:IF:204:HIS:CB | 12:IF:210:PRO:HA | 2.40 | 0.52 |
| 5:K:193:VAL:O | 5:K:199:GLU:N | 2.37 | 0.52 |
| 5:J:308:SER:HG | 5:K:258:TYR:HD2 | 1.58 | 0.52 |
| 7:Q:167:GLN:O | 7:Q:171:LYS:HG2 | 2.10 | 0.52 |
| 8:R:50:PRO:HB2 | 8:R:57:LYS:HD3 | 1.91 | 0.52 |
| 8:R:72:THR:HA | 8:R:154:GLU:HA | 1.92 | 0.52 |
| 1:X:238:PHE:HE1 | 1:X:262:PRO:HD2 | 1.73 | 0.52 |
| 1:X:543:THR:CG2 | 1:X:552:LYS:H | 2.23 | 0.52 |
| 1:X:508:ARG:NH2 | 1:X:576:ASP:O | 2.42 | 0.52 |
| 1:Y:519:SER:HB3 | 1:Y:533:ASP:OD2 | 2.09 | 0.52 |
| 13:YA:116[B]:ASP:OD2 | 13:YA:121[B]:TYR:N | 2.42 | 0.52 |
| 13:YA:321[D]:LYS:HD3 | 13:YB:452[D]:GLY:CA | 2.34 | 0.52 |
| 13:YA:461[E]:SER:OG | 13:YC:468[E]:ASP:OD2 | 2.27 | 0.52 |
| 13:YB:379[F]:PRO:HG2 | 13:YB:429[F]:ARG:CZ | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:436[C]:ASP:OD2 | 13:YB:437[C]:ASN:N | 2.43 | 0.52 |
| 13:YB:460[C]:GLY:N | 13:YC:452[C]:GLY:O | 2.42 | 0.52 |
| 13:YB:61[C]:ILE:HA | 13:YC:76[C]:PRO:CA | 2.39 | 0.52 |
| 13:YC:116[E]:ASP:OD2 | 13:YC:121[E]:TYR:N | 2.42 | 0.52 |
| 13:YC:193[E]:ASP:OD1 | 13:YC:197[E]:TYR:N | 2.33 | 0.52 |
| 13:YB:18[A]:ARG:HG3 | 13:YC:388[A]:PRO:HG3 | 1.91 | 0.52 |
| 13:YB:18[C]:ARG:HG3 | 13:YC:388[C]:PRO:HG3 | 1.92 | 0.52 |
| 13:YC:379[F]:PRO:HG2 | 13:YC:429[F]:ARG:CZ | 2.40 | 0.52 |
| 13:YC:436[F]:ASP:OD2 | 13:YC:437[F]:ASN:N | 2.43 | 0.52 |
| 13:YA:565[E]:TYR:CE2 | 13:YC:567[E]:ILE:HG23 | 2.44 | 0.52 |
| 14:YD:330[F]:LYS:HA | 14:YD:330[F]:LYS:HE3 | 1.91 | 0.52 |
| 14:YD:360[A]:ASN:N | 14:YD:360[A]:ASN:HD22 | 1.98 | 0.52 |
| 14:YD:332[D]:GLN:OE1 | 14:YE:101[D]:GLY:HA2 | 2.10 | 0.52 |
| 14:YE:172[A]:TYR:CE1 | 14:YE:176[A]:VAL:HG21 | 2.45 | 0.52 |
| 14:YE:330[A]:LYS:HA | 14:YE:330[A]:LYS:HE3 | 1.91 | 0.52 |
| 14:YF:124[F]:PHE:CE2 | 14:YF:135[F]:MET:HE2 | 2.44 | 0.52 |
| 14:YD:92[D]:HIS:NE2 | 14:YF:238[D]:THR:OG1 | 2.43 | 0.52 |
| 14:YF:278[A]:SER:O | 14:YF:279[A]:ARG:NH1 | 2.41 | 0.52 |
| 2:Z:646:ARG:CD | 2:Z:673:GLN:HE22 | 2.13 | 0.52 |
| 1:A:543:THR:CG2 | 1:A:552:LYS:H | 2.23 | 0.52 |
| 4:AA:204:VAL:HG22 | 4:AA:276:VAL:HG22 | 1.92 | 0.52 |
| 5:AD:180:VAL:HG13 | 5:AD:181:PHE:N | 2.25 | 0.52 |
| 5:AE:102:TRP:HB2 | 5:AE:129:ARG:O | 2.10 | 0.52 |
| 5:AE:305:ASN:OD1 | 5:AE:305:ASN:N | 2.42 | 0.52 |
| 5:AE:319:GLU:OE2 | 5:AE:324:VAL:HG13 | 2.10 | 0.52 |
| 5:AE:31:ASP:O | 5:AE:35:TYR:N | 2.27 | 0.52 |
| 5:AE:290:SER:HB3 | 5:AE:371:PHE:H | 1.75 | 0.52 |
| 5:AE:54:ALA:HB2 | 5:AE:71:ASN:O | 2.09 | 0.52 |
| 6:AF:195:LEU:HD13 | 6:AF:215:PHE:HE1 | 1.74 | 0.52 |
| 5:AE:316:ILE:HD11 | 6:AF:7:LYS:NZ | 2.25 | 0.52 |
| 7:AI:480:ARG:NE | 7:AJ:465:ARG:HG3 | 2.25 | 0.52 |
| 7:AI:45:ASN:CG | 7:AJ:24:ASN:HD21 | 2.14 | 0.52 |
| 8:BC:36:CYS:HA | 8:BC:73:VAL:HG12 | 1.91 | 0.52 |
| 9:BD:125:GLN:OE1 | 9:BD:125:GLN:N | 2.43 | 0.52 |
| 12:BG:216:PHE:HE1 | 12:BG:218:MET:CE | 2.23 | 0.52 |
| 1:BH:174:ARG:NH2 | 1:BH:269:VAL:HG21 | 2.25 | 0.52 |
| 1:BH:627:PRO:HG3 | 1:BH:632:ILE:HD11 | 1.92 | 0.52 |
| 1:BI:112:LEU:HB3 | 1:BI:300:ILE:HG22 | 1.92 | 0.52 |
| 2:BJ:514:PHE:CD1 | 2:BJ:525:TRP:HB2 | 2.45 | 0.52 |
| 1:BI:55:VAL:HG21 | 2:BJ:657:TYR:CE1 | 2.45 | 0.52 |
| 2:C:782:VAL:HA | 2:C:795:VAL:HG23 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:969:TYR:HD2 | 2:C:982:LEU:HD13 | 1.75 | 0.52 |
| 1:BH:635:ARG:NH2 | 3:CB:322:MET:SD | 2.83 | 0.52 |
| 5:CG:110:VAL:HG22 | 5:CG:123:PRO:HB3 | 1.92 | 0.52 |
| 5:CG:191:ILE:H | 5:CH:164:ARG:HH21 | 1.58 | 0.52 |
| 5:CG:323:THR:CG2 | 5:CG:359:GLU:HB2 | 2.39 | 0.52 |
| 5:CG:501:LEU:HB3 | 5:CG:512:PRO:HB2 | 1.91 | 0.52 |
| 5:CG:308:SER:HG | 5:CH:258:TYR:HD2 | 1.57 | 0.52 |
| 3:D:24:PHE:O | 3:D:27:SER:OG | 2.19 | 0.52 |
| 7:DB:171:LYS:O | 7:DB:175:GLN:N | 2.43 | 0.52 |
| 7:DB:511:GLU:HB3 | 7:DB:513:ARG:HH11 | 1.74 | 0.52 |
| 7:DB:76:VAL:HG11 | 7:DD:81:LEU:HD22 | 1.92 | 0.52 |
| 7:DC:47:VAL:HG12 | 7:DC:48:PRO:N | 2.24 | 0.52 |
| 9:DG:75:ARG:HG3 | 10:DH:123:PRO:HG3 | 1.92 | 0.52 |
| 1:EA:444:ILE:O | 1:EA:447:TYR:N | 2.43 | 0.52 |
| 2:EC:106:ASN:OD1 | 2:EC:107:ALA:N | 2.43 | 0.52 |
| 2:EC:120:ASN:CB | 2:EC:155:PRO:HB3 | 2.35 | 0.52 |
| 2:EC:433:ASN:HD21 | 2:EC:513:PHE:HA | 1.75 | 0.52 |
| 2:EC:701:TRP:CD2 | 2:EC:701:TRP:O | 2.64 | 0.52 |
| 2:EC:853:ASP:HB2 | 2:EC:855:ILE:HG22 | 1.92 | 0.52 |
| 4:EF:131:LYS:HD3 | 4:EF:161:ASN:ND2 | 2.25 | 0.52 |
| 5:EI:102:TRP:HB2 | 5:EI:129:ARG:O | 2.10 | 0.52 |
| 5:EI:264:ARG:HG3 | 5:EI:379:ASP:O | 2.10 | 0.52 |
| 5:EI:64:TRP:O | 5:EI:93:ILE:HG22 | 2.10 | 0.52 |
| 5:FA:354:THR:HG22 | 5:FA:372:ASP:CG | 2.30 | 0.52 |
| 6:FB:14:LEU:O | 6:FB:16:ASP:N | 2.43 | 0.52 |
| 6:FC:14:LEU:O | 6:FC:16:ASP:N | 2.43 | 0.52 |
| 7:FE:202:GLY:HA3 | 7:FG:216:MET:SD | 2.50 | 0.52 |
| 7:FF:463:THR:HG21 | 7:FG:490:ILE:HD12 | 1.91 | 0.52 |
| 8:FI:72:THR:HA | 8:FI:154:GLU:HA | 1.92 | 0.52 |
| 12:GC:216:PHE:HE1 | 12:GC:218:MET:CE | 2.23 | 0.52 |
| 2:GF:138:ASN:OD1 | 2:GF:139:ASN:ND2 | 2.42 | 0.52 |
| 2:GF:183:VAL:HA | 2:GF:210:LYS:HE3 | 1.91 | 0.52 |
| 2:GF:180:ILE:HA | 2:GF:219:TRP:CH2 | 2.45 | 0.52 |
| 2:GF:416:VAL:HG23 | 2:GF:417:PHE:N | 2.25 | 0.52 |
| 4:GI:131:LYS:HD3 | 4:GI:161:ASN:ND2 | 2.25 | 0.52 |
| 5:HB:118:LYS:NZ | 5:HB:145:TYR:O | 2.36 | 0.52 |
| 5:HB:320:LEU:HG | 5:HB:357:SER:HB3 | 1.92 | 0.52 |
| 5:HC:357:SER:OG | 6:HE:4:LEU:HD21 | 2.10 | 0.52 |
| 5:HD:319:GLU:OE2 | 5:HD:324:VAL:HG13 | 2.10 | 0.52 |
| 7:HH:265:LEU:O | 7:HI:257:THR:HA | 2.09 | 0.52 |
| 7:HH:32:VAL:O | 7:HH:36:ILE:N | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:220:SER:OG | 7:HI:226:GLY:O | 2.28 | 0.52 |
| 5:I:194:LYS:HB2 | 5:I:243:GLN:HB2 | 1.92 | 0.52 |
| 10:ID:323:LYS:HB3 | 10:ID:339:PRO:HG3 | 1.92 | 0.52 |
| 5:J:289:LYS:O | 5:J:290:SER:OG | 2.25 | 0.52 |
| 6:M:82:VAL:HB | 6:M:187:LYS:HB3 | 1.92 | 0.52 |
| 7:O:451:PHE:HD1 | 7:O:469:VAL:HG13 | 1.75 | 0.52 |
| 7:O:54:THR:HG22 | 7:O:55:LYS:O | 2.10 | 0.52 |
| 7:P:20:PRO:HG3 | 7:P:29:ILE:HG13 | 1.91 | 0.52 |
| 7:Q:255:SER:HB3 | 7:Q:263:VAL:CG1 | 2.40 | 0.52 |
| 7:Q:20:PRO:HD3 | 7:Q:29:ILE:HG21 | 1.92 | 0.52 |
| 8:S:50:PRO:HB2 | 8:S:57:LYS:HD3 | 1.91 | 0.52 |
| 8:S:5:ASP:OD1 | 8:S:8:ARG:NH1 | 2.43 | 0.52 |
| 12:W:125:ILE:HA | 12:W:162:PHE:CB | 2.39 | 0.52 |
| 1:Y:112:LEU:HB3 | 1:Y:300:ILE:HG22 | 1.92 | 0.52 |
| 1:Y:448:TYR:CD1 | 1:Y:452:VAL:HG11 | 2.44 | 0.52 |
| 1:Y:619:GLN:OE1 | 1:Y:619:GLN:N | 2.35 | 0.52 |
| 13:YA:16[C]:GLU:OE2 | 13:YA:39[C]:ARG:NH2 | 2.42 | 0.52 |
| 13:YA:66[B]:MET:O | 13:YA:69[B]:ILE:N | 2.43 | 0.52 |
| 13:YA:481[B]:PHE:O | 13:YB:473[B]:GLN:HA | 2.09 | 0.52 |
| 13:YA:481[C]:PHE:O | 13:YB:473[C]:GLN:HA | 2.09 | 0.52 |
| 13:YC:379[E]:PRO:HG2 | 13:YC:429[E]:ARG:CZ | 2.40 | 0.52 |
| 13:YB:554[A]:MET:HG3 | 13:YC:550[A]:TRP:HB2 | 1.91 | 0.52 |
| 14:YD:232[A]:TYR:HD2 | 14:YD:233[A]:ASP:OD1 | 1.92 | 0.52 |
| 14:YE:124[B]:PHE:CE2 | 14:YE:135[B]:MET:HE2 | 2.44 | 0.52 |
| 14:YE:278[B]:SER:O | 14:YE:279[B]:ARG:NH1 | 2.42 | 0.52 |
| 14:YE:230[D]:LEU:HB2 | 14:YE:313[D]:ILE:HD11 | 1.91 | 0.52 |
| 14:YE:330[B]:LYS:HA | 14:YE:330[B]:LYS:HE3 | 1.91 | 0.52 |
| 14:YE:73[B]:SER:OG | 14:YE:85[B]:THR:OG1 | 2.27 | 0.52 |
| 14:YF:172[F]:TYR:CE1 | 14:YF:176[F]:VAL:HG21 | 2.45 | 0.52 |
| 14:YF:172[A]:TYR:CE1 | 14:YF:176[A]:VAL:HG21 | 2.45 | 0.52 |
| 14:YF:230[E]:LEU:HB2 | 14:YF:313[E]:ILE:HD11 | 1.91 | 0.52 |
| 2:Z:172:GLU:HA | 4:AA:166:SER:H | 90.21 | 0.52 |
| 2:Z:180:ILE:HA | 2:Z:219:TRP:CH2 | 2.45 | 0.52 |
| 2:Z:233:LEU:HD23 | 2:Z:234:SER:OG | 2.10 | 0.52 |
| 2:Z:572:ASN:HB3 | 2:Z:611:ILE:HG22 | 1.92 | 0.52 |
| 1:Y:402:ALA:HB2 | 2:Z:741:GLU:HA | 1.92 | 0.52 |
| 1:A:238:PHE:HE1 | 1:A:262:PRO:HD2 | 1.73 | 0.51 |
| 5:AC:102:TRP:HB2 | 5:AC:129:ARG:O | 2.10 | 0.51 |
| 5:AC:79:ILE:HG13 | 5:AC:108:THR:O | 2.10 | 0.51 |
| 5:AE:204:ASP:OD1 | 5:AE:205:VAL:N | 2.43 | 0.51 |
| 5:AE:223:VAL:HB | 5:AE:224:PRO:HD3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:356:TYR:HE1 | 6:AG:4:LEU:HD13 | 1.76 | 0.51 |
| 7:AI:49:ASP:O | 7:AI:56:GLY:HA3 | 2.09 | 0.51 |
| 7:AJ:367:VAL:O | 7:AJ:389:ASN:HA | 2.10 | 0.51 |
| 7:AJ:466:SER:HB3 | 7:AJ:468:PHE:CE2 | 2.45 | 0.51 |
| 1:B:156:ASP:HB3 | 1:B:160:GLN:O | 2.10 | 0.51 |
| 1:B:538:VAL:HG11 | 1:B:558:PHE:CE1 | 2.45 | 0.51 |
| 1:BI:547:SER:O | 1:BI:548:LYS:HG2 | 2.10 | 0.51 |
| 2:BJ:149:GLU:O | 2:BJ:150:SER:OG | 2.18 | 0.51 |
| 2:BJ:58:ASN:HB3 | 4:CD:155:ASN:HD21 | 1.74 | 0.51 |
| 3:CB:137:PRO:HG3 | 3:CB:185:GLY:HA3 | 1.92 | 0.51 |
| 3:CB:221:THR:O | 3:CB:224:GLY:N | 2.37 | 0.51 |
| 4:CE:131:LYS:HD3 | 4:CE:161:ASN:ND2 | 2.25 | 0.51 |
| 5:CF:64:TRP:CE2 | 5:CF:82:PRO:HG2 | 2.44 | 0.51 |
| 5:CG:89:TYR:CD1 | 5:CG:139:ALA:HA | 2.45 | 0.51 |
| 5:CG:86:VAL:HG22 | 5:CG:87:ASN:H | 1.74 | 0.51 |
| 5:CH:356:TYR:CE1 | 6:CJ:4:LEU:HD13 | 2.45 | 0.51 |
| 3:D:279:LEU:HD12 | 3:E:232:GLN:HE21 | 1.75 | 0.51 |
| 7:DB:349:TRP:CZ3 | 7:DC:342:PRO:HG2 | 2.45 | 0.51 |
| 7:DC:511:GLU:HB3 | 7:DC:513:ARG:NH1 | 2.25 | 0.51 |
| 7:DC:99:ARG:HD3 | 7:DC:111:ASN:ND2 | 2.20 | 0.51 |
| 10:DH:205:LYS:HB2 | 10:DH:311:PHE:HZ | 1.74 | 0.51 |
| 1:EA:286:PHE:HB2 | 1:EA:300:ILE:CD1 | 2.39 | 0.51 |
| 1:EB:348:PHE:CZ | 1:EB:399:TYR:CD2 | 2.98 | 0.51 |
| 1:EB:443:LYS:HG2 | 1:EB:471:ALA:HB2 | 1.92 | 0.51 |
| 2:EC:107:ALA:HB2 | 2:EC:128:THR:HA | 1.90 | 0.51 |
| 2:EC:351:GLU:CB | 2:EC:353:ASP:HB2 | 2.31 | 0.51 |
| 2:EC:572:ASN:HB3 | 2:EC:611:ILE:HG22 | 1.92 | 0.51 |
| 5:EI:257:SER:OG | 5:EI:387:ASN:HB2 | 2.09 | 0.51 |
| 5:EI:49:TRP:CD1 | 5:EI:67:SER:HB3 | 2.44 | 0.51 |
| 5:FA:193:VAL:O | 5:FA:199:GLU:N | 2.38 | 0.51 |
| 5:FA:290:SER:HB3 | 5:FA:371:PHE:H | 1.75 | 0.51 |
| 5:EI:488:VAL:HG22 | 5:FA:486:VAL:HG12 | 1.91 | 0.51 |
| 6:FC:54:SER:O | 6:FD:164:GLN:NE2 | 2.43 | 0.51 |
| 6:FD:14:LEU:O | 6:FD:16:ASP:N | 2.43 | 0.51 |
| 7:FE:322:THR:HG23 | 7:FF:327:GLN:HE21 | 1.75 | 0.51 |
| 7:FE:100:TYR:OH | 7:FF:113:GLU:HG3 | 2.09 | 0.51 |
| 7:FF:451:PHE:CE1 | 7:FF:470:GLY:HA2 | 2.46 | 0.51 |
| 7:FF:472:ARG:HG3 | 7:FF:473:LYS:HG3 | 1.92 | 0.51 |
| 7:FF:511:GLU:HB3 | 7:FF:513:ARG:NH1 | 2.25 | 0.51 |
| 7:FG:255:SER:HB3 | 7:FG:263:VAL:CG1 | 2.40 | 0.51 |
| 11:GB:73:LEU:HD22 | 11:GB:86:TRP:HH2 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:GC:224:SER:HB3 | 12:GC:240:ASP:OD1 | 2.11 | 0.51 |
| 1:GD:508:ARG:NH2 | 1:GD:576:ASP:O | 2.42 | 0.51 |
| 1:GE:348:PHE:CZ | 1:GE:399:TYR:CD2 | 2.99 | 0.51 |
| 2:GF:379:ILE:HG13 | 2:GF:402:GLY:O | 2.11 | 0.51 |
| 2:GF:380:ILE:O | 2:GF:401:LYS:HD2 | 2.10 | 0.51 |
| 2:GF:992:PRO:HB3 | 5:HD:19:LEU:HB3 | 1.92 | 0.51 |
| 3:GG:226:GLU:N | 3:GG:226:GLU:OE1 | 2.34 | 0.51 |
| 3:GH:137:PRO:HG3 | 3:GH:185:GLY:HA3 | 1.92 | 0.51 |
| 3:GH:202:ARG:O | 3:GH:248:ARG:NH1 | 2.42 | 0.51 |
| 5:HB:51:THR:HA | 5:HB:69:ALA:HB3 | 1.92 | 0.51 |
| 5:HC:110:VAL:HG22 | 5:HC:123:PRO:HB3 | 1.92 | 0.51 |
| 5:HC:410:GLN:HG2 | 5:HC:443:PHE:O | 2.10 | 0.51 |
| 5:HD:354:THR:HG22 | 5:HD:372:ASP:CG | 2.30 | 0.51 |
| 7:HI:119:ALA:O | 7:HI:122:THR:OG1 | 2.24 | 0.51 |
| 7:HI:406:GLY:O | 7:HI:410:THR:HG23 | 2.10 | 0.51 |
| 5:I:208:GLU:OE1 | 5:I:233:ARG:NH2 | 2.43 | 0.51 |
| 5:J:180:VAL:HG13 | 5:J:181:PHE:N | 2.25 | 0.51 |
| 5:K:102:TRP:HB2 | 5:K:129:ARG:O | 2.10 | 0.51 |
| 6:M:195:LEU:HD13 | 6:M:215:PHE:HE1 | 1.74 | 0.51 |
| 5:K:356:TYR:HE1 | 6:M:4:LEU:HD13 | 1.75 | 0.51 |
| 7:O:99:ARG:NH1 | 7:O:105:GLU:OE2 | 2.32 | 0.51 |
| 7:O:72:ASN:HA | 7:Q:77:THR:HG21 | 1.91 | 0.51 |
| 7:P:110:VAL:HG12 | 7:P:111:ASN:H | 1.74 | 0.51 |
| 7:Q:34:ALA:HA | 7:Q:37:ALA:HB3 | 1.91 | 0.51 |
| 9:T:125:GLN:OE1 | 9:T:125:GLN:N | 2.43 | 0.51 |
| 11:V:31:ASN:OD1 | 11:V:32:TYR:N | 2.41 | 0.51 |
| 11:V:73:LEU:HD22 | 11:V:86:TRP:HH2 | 1.75 | 0.51 |
| 12:W:30:PRO:HG3 | 12:W:197:ALA:HB2 | 1.92 | 0.51 |
| 1:X:619:GLN:HG2 | 1:X:620:THR:HG23 | 1.92 | 0.51 |
| 13:YA:441[B]:ILE:HG21 | 13:YB:378[B]:GLU:OE2 | 2.10 | 0.51 |
| 13:YA:61[F]:ILE:HG12 | 13:YB:60[F]:PRO:HD2 | 1.92 | 0.51 |
| 13:YC:256[C]:ILE:HA | 13:YC:286[C]:VAL:HG21 | 1.92 | 0.51 |
| 13:YA:59[A]:GLN:CA | 13:YC:61[A]:ILE:HG21 | 2.31 | 0.51 |
| 14:YD:360[A]:ASN:ND2 | 14:YD:360[A]:ASN:H | 2.04 | 0.51 |
| 14:YE:172[B]:TYR:CE1 | 14:YE:176[B]:VAL:HG21 | 2.45 | 0.51 |
| 14:YE:230[E]:LEU:HB2 | 14:YE:313[E]:ILE:HD11 | 1.91 | 0.51 |
| 14:YE:238[C]:THR:OG1 | 14:YF:92[C]:HIS:NE2 | 2.43 | 0.51 |
| 14:YE:230[B]:LEU:HB2 | 14:YE:313[B]:ILE:HD11 | 1.91 | 0.51 |
| 11:V:182:ASN:ND2 | 14:YE:327[E]:ASN:HD22 | 2.08 | 0.51 |
| 14:YE:330[C]:LYS:HE3 | 14:YE:330[C]:LYS:HA | 1.91 | 0.51 |
| 14:YD:332[C]:GLN:HB3 | 14:YE:61[C]:HIS:NE2 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:332[F]:GLN:OE1 | 14:YF:101[F]:GLY:HA2 | 2.10 | 0.51 |
| 14:YF:124[B]:PHE:CE2 | 14:YF:135[B]:MET:HE2 | 2.45 | 0.51 |
| 14:YF:172[E]:TYR:CE1 | 14:YF:176[E]:VAL:HG21 | 2.45 | 0.51 |
| 2:Z:12:ARG:HG3 | 2:Z:24:ARG:HB2 | 1.92 | 0.51 |
| 1:A:18:PRO:O | 1:A:19:GLU:HG2 | 2.10 | 0.51 |
| 1:A:444:ILE:O | 1:A:447:TYR:N | 2.43 | 0.51 |
| 5:AC:172:GLN:HG2 | 5:AC:173:GLY:H | 1.75 | 0.51 |
| 5:AC:1:MET:H3 | 5:AD:41:ASP:HB3 | 1.75 | 0.51 |
| 5:AD:110:VAL:HG22 | 5:AD:123:PRO:HB3 | 1.92 | 0.51 |
| 6:AH:195:LEU:HD13 | 6:AH:215:PHE:HE1 | 1.74 | 0.51 |
| 7:AI:100:TYR:OH | 7:AJ:113:GLU:HG3 | 2.09 | 0.51 |
| 7:AI:54:THR:HG22 | 7:AI:55:LYS:O | 2.10 | 0.51 |
| 1:B:348:PHE:CZ | 1:B:399:TYR:CD2 | 2.99 | 0.51 |
| 1:B:448:TYR:CD1 | 1:B:452:VAL:HG11 | 2.44 | 0.51 |
| 10:BE:132:SER:OG | 10:BE:135:ASP:HB2 | 2.08 | 0.51 |
| 10:BE:143:PHE:CE2 | 10:DH:349:ARG:HD3 | 2.45 | 0.51 |
| 11:BF:30:ARG:HH12 | 11:BF:192:TYR:HD1 | 1.57 | 0.51 |
| 12:BG:144:ASN:ND2 | 10:DH:57:LEU:HG | 2.25 | 0.51 |
| 1:BH:208:ASN:ND2 | 1:BH:224:TYR:OH | 2.44 | 0.51 |
| 2:BJ:449:LYS:HD2 | 3:ED:74:HIS:NE2 | 2.26 | 0.51 |
| 2:BJ:934:ALA:HB1 | 2:BJ:942:ILE:HD12 | 1.91 | 0.51 |
| 2:C:379:ILE:HG13 | 2:C:402:GLY:O | 2.11 | 0.51 |
| 2:C:7:SER:O | 2:C:28:VAL:HG11 | 2.09 | 0.51 |
| 4:CC:131:LYS:HD3 | 4:CC:161:ASN:ND2 | 2.25 | 0.51 |
| 4:CC:284:ILE:HD11 | 4:CE:205:THR:HG22 | 1.91 | 0.51 |
| 5:CF:49:TRP:CD1 | 5:CF:67:SER:HB3 | 2.44 | 0.51 |
| 5:CG:89:TYR:CE1 | 5:CG:139:ALA:HA | 2.44 | 0.51 |
| 5:CH:362:GLU:HB2 | 5:CH:365:ILE:O | 2.09 | 0.51 |
| 5:CH:78:THR:HA | 5:CH:108:THR:HB | 1.92 | 0.51 |
| 5:CG:318:GLN:HB3 | 6:CI:4:LEU:HG | 1.91 | 0.51 |
| 6:CJ:82:VAL:HB | 6:CJ:187:LYS:HB3 | 1.92 | 0.51 |
| 3:D:23:ASN:OD1 | 3:E:27:SER:OG | 2.18 | 0.51 |
| 7:DB:211:SER:O | 7:DB:215:PHE:N | 2.43 | 0.51 |
| 12:DJ:15:ASP:OD1 | 12:DJ:16:PHE:N | 2.44 | 0.51 |
| 1:EB:105:ALA:HB2 | 1:EB:275:THR:HG21 | 1.92 | 0.51 |
| 1:EB:547:SER:O | 1:EB:548:LYS:HG2 | 2.10 | 0.51 |
| 1:EB:65:LEU:HD21 | 11:GB:70:TYR:OH | 2.09 | 0.51 |
| 2:EC:154:SER:OG | 2:EC:156:SER:OG | 2.13 | 0.51 |
| 2:EC:225:PHE:CE1 | 2:EC:294:PHE:HD2 | 2.29 | 0.51 |
| 2:EC:416:VAL:HG23 | 2:EC:417:PHE:N | 2.25 | 0.51 |
| 2:EC:782:VAL:HA | 2:EC:795:VAL:HG23 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:104:TYR:HE2 | 3:ED:165:ARG:NH2 | 2.08 | 0.51 |
| 4:EF:204:VAL:HG22 | 4:EF:276:VAL:HG22 | 1.92 | 0.51 |
| 4:EF:205:THR:HG22 | 4:EG:284:ILE:HD11 | 1.92 | 0.51 |
| 4:EF:7:LYS:HD3 | 4:EH:39:TYR:CG | 2.45 | 0.51 |
| 4:EH:131:LYS:HD3 | 4:EH:161:ASN:ND2 | 2.25 | 0.51 |
| 4:EF:201:LYS:NZ | 4:EH:218:GLU:OE1 | 2.31 | 0.51 |
| 5:EI:208:GLU:OE1 | 5:EI:233:ARG:NH2 | 2.43 | 0.51 |
| 5:EI:241:THR:HG21 | 5:FA:200:LEU:CD1 | 2.40 | 0.51 |
| 5:EI:289:LYS:HE2 | 5:EI:370:HIS:HE1 | 1.74 | 0.51 |
| 4:F:107:VAL:O | 4:F:148:LEU:N | 2.39 | 0.51 |
| 5:FA:305:ASN:OD1 | 5:FA:305:ASN:N | 2.42 | 0.51 |
| 5:FA:362:GLU:HB2 | 5:FA:365:ILE:O | 2.09 | 0.51 |
| 5:FA:397:ASP:O | 5:FA:400:ILE:HG22 | 2.10 | 0.51 |
| 7:FE:451:PHE:HD1 | 7:FE:469:VAL:HG13 | 1.75 | 0.51 |
| 7:FF:20:PRO:HG3 | 7:FF:29:ILE:HG13 | 1.91 | 0.51 |
| 7:FF:43:GLY:O | 7:FG:42:ALA:HB3 | 2.09 | 0.51 |
| 7:FG:375:TYR:CE2 | 7:FG:390:PRO:HB2 | 2.45 | 0.51 |
| 8:FI:5:ASP:OD1 | 8:FI:8:ARG:NH1 | 2.43 | 0.51 |
| 4:F:172:GLU:HA | 4:G:166:SER:H | 1.74 | 0.51 |
| 12:GC:211:HIS:HE1 | 12:IF:167:GLU:HA | 1.75 | 0.51 |
| 12:GC:223:VAL:HA | 12:GC:241:VAL:HA | 1.92 | 0.51 |
| 1:GD:18:PRO:O | 1:GD:19:GLU:HG2 | 2.10 | 0.51 |
| 1:GD:208:ASN:ND2 | 1:GD:224:TYR:OH | 2.44 | 0.51 |
| 1:GD:174:ARG:NH2 | 1:GD:269:VAL:HG21 | 2.25 | 0.51 |
| 1:GD:286:PHE:HB2 | 1:GD:300:ILE:CD1 | 2.39 | 0.51 |
| 1:GE:112:LEU:HB3 | 1:GE:300:ILE:HG22 | 1.92 | 0.51 |
| 2:GF:231:TYR:HE2 | 2:GF:389:ASN:HD21 | 1.58 | 0.51 |
| 2:GF:433:ASN:HD21 | 2:GF:513:PHE:HA | 1.75 | 0.51 |
| 3:D:65:VAL:HG13 | 2:GF:486:HIS:HD2 | 1.75 | 0.51 |
| 2:GF:969:TYR:O | 2:GF:973:ASN:N | 2.29 | 0.51 |
| 3:GG:289:ASN:HD21 | 3:GH:233:GLN:HB2 | 1.75 | 0.51 |
| 3:GG:313:GLU:HG3 | 3:GH:10:ALA:HB2 | 1.92 | 0.51 |
| 4:GJ:218:GLU:OE1 | 4:HA:201:LYS:NZ | 2.35 | 0.51 |
| 5:HB:175:THR:O | 5:HB:232:LEU:N | 2.35 | 0.51 |
| 5:HC:289:LYS:O | 5:HC:290:SER:OG | 2.25 | 0.51 |
| 5:HD:223:VAL:HB | 5:HD:224:PRO:HD3 | 1.92 | 0.51 |
| 5:HD:290:SER:HB3 | 5:HD:371:PHE:H | 1.75 | 0.51 |
| 5:HD:72:THR:HG22 | 5:HD:77:VAL:HG22 | 1.92 | 0.51 |
| 7:HI:78:PRO:HB2 | 7:HJ:69:GLY:HA2 | 1.92 | 0.51 |
| 7:HJ:365:GLY:O | 7:HJ:392:LEU:N | 2.25 | 0.51 |
| 7:HH:452:GLY:HA3 | 7:HJ:480:ARG:O | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:72:ASN:HA | 7:HJ:77:THR:HG21 | 1.92 | 0.51 |
| 5:I:361:ASP:OD1 | 5:I:362:GLU:N | 2.43 | 0.51 |
| 5:I:488:VAL:HG22 | 5:K:486:VAL:HG12 | 1.91 | 0.51 |
| 5:I:51:THR:HA | 5:I:69:ALA:HB3 | 1.92 | 0.51 |
| 5:I:64:TRP:O | 5:I:93:ILE:HG22 | 2.10 | 0.51 |
| 8:IA:36:CYS:HA | 8:IA:73:VAL:HG12 | 1.91 | 0.51 |
| 5:J:110:VAL:HG22 | 5:J:123:PRO:HB3 | 1.92 | 0.51 |
| 5:K:362:GLU:HB2 | 5:K:365:ILE:O | 2.09 | 0.51 |
| 5:I:49:TRP:C | 5:K:90:ASN:HD21 | 2.11 | 0.51 |
| 6:L:14:LEU:O | 6:L:16:ASP:N | 2.43 | 0.51 |
| 7:O:246:THR:HG1 | 7:O:249:THR:H | 1.59 | 0.51 |
| 7:P:220:SER:OG | 7:P:226:GLY:O | 2.28 | 0.51 |
| 7:P:36:ILE:HG13 | 7:Q:18:PHE:CE1 | 2.46 | 0.51 |
| 9:T:61:LEU:HG | 9:T:69:THR:HG23 | 1.91 | 0.51 |
| 13:YA:116[F]:ASP:OD2 | 13:YA:121[F]:TYR:N | 2.43 | 0.51 |
| 13:YA:256[C]:ILE:HA | 13:YA:286[C]:VAL:HG21 | 1.92 | 0.51 |
| 13:YA:442[E]:THR:HA | 13:YB:434[E]:THR:O | 2.09 | 0.51 |
| 13:YB:18[B]:ARG:HG3 | 13:YC:388[B]:PRO:HG3 | 1.92 | 0.51 |
| 13:YA:520[C]:THR:O | 13:YC:529[C]:THR:N | 2.42 | 0.51 |
| 14:YD:172[A]:TYR:CE1 | 14:YD:176[A]:VAL:HG21 | 2.45 | 0.51 |
| 14:YD:172[B]:TYR:CE1 | 14:YD:176[B]:VAL:HG21 | 2.45 | 0.51 |
| 14:YE:172[C]:TYR:CE1 | 14:YE:176[C]:VAL:HG21 | 2.45 | 0.51 |
| 14:YE:172[F]:TYR:CE1 | 14:YE:176[F]:VAL:HG21 | 2.45 | 0.51 |
| 14:YE:278[F]:SER:O | 14:YE:279[F]:ARG:NH1 | 2.41 | 0.51 |
| 14:YF:330[C]:LYS:HE3 | 14:YF:330[C]:LYS:HA | 1.91 | 0.51 |
| 2:Z:494:GLU:HG3 | 2:Z:498:TRP:CD2 | 2.44 | 0.51 |
| 15:ZA:76[E]:GLN:HB3 | 15:ZA:96[E]:ILE:HD11 | 1.91 | 0.51 |
| 4:AA:27:GLY:HA2 | 4:AA:30:LYS:HD2 | 1.91 | 0.51 |
| 5:AC:144:GLU:OE1 | 5:AC:144:GLU:N | 2.43 | 0.51 |
| 5:AC:268:SER:N | 5:AC:283:THR:O | 2.35 | 0.51 |
| 5:AC:86:VAL:HG22 | 5:AC:87:ASN:H | 1.76 | 0.51 |
| 5:AD:89:TYR:CD1 | 5:AD:139:ALA:HA | 2.45 | 0.51 |
| 5:AD:569:TYR:HE1 | 5:AE:544:VAL:HG22 | 1.74 | 0.51 |
| 5:AE:192:ARG:HG3 | 5:AE:245:GLU:HB2 | 1.93 | 0.51 |
| 5:AE:323:THR:HG21 | 5:AE:354:THR:HG23 | 1.91 | 0.51 |
| 6:AH:14:LEU:O | 6:AH:16:ASP:N | 2.43 | 0.51 |
| 7:AJ:511:GLU:HB3 | 7:AJ:513:ARG:NH1 | 2.25 | 0.51 |
| 1:BH:87:SER:OG | 1:BH:230:ILE:O | 2.21 | 0.51 |
| 1:BH:69:GLN:HE21 | 11:DI:25:MET:CE | 2.23 | 0.51 |
| 1:BI:443:LYS:HG2 | 1:BI:471:ALA:HB2 | 1.92 | 0.51 |
| 2:BJ:371:ILE:HG13 | 2:BJ:372:CYS:H | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:788:THR:HG23 | 2:C:790:THR:N | 2.24 | 0.51 |
| 4:CC:53:GLY:O | 4:CD:7:LYS:HB3 | 2.10 | 0.51 |
| 5:CF:264:ARG:HG3 | 5:CF:379:ASP:O | 2.10 | 0.51 |
| 5:CH:223:VAL:HB | 5:CH:224:PRO:HD3 | 1.93 | 0.51 |
| 5:CH:319:GLU:OE2 | 5:CH:324:VAL:HG13 | 2.10 | 0.51 |
| 6:CI:82:VAL:HB | 6:CI:187:LYS:HB3 | 1.92 | 0.51 |
| 6:DA:14:LEU:O | 6:DA:16:ASP:N | 2.43 | 0.51 |
| 7:DB:485:ASN:C | 7:DC:446:LYS:HG2 | 2.30 | 0.51 |
| 7:DC:472:ARG:HG3 | 7:DC:473:LYS:HG3 | 1.92 | 0.51 |
| 7:DC:399:PHE:HZ | 7:DC:516:ASN:HD22 | 1.58 | 0.51 |
| 9:DG:125:GLN:N | 9:DG:125:GLN:OE1 | 2.43 | 0.51 |
| 1:EA:208:ASN:ND2 | 1:EA:224:TYR:OH | 2.44 | 0.51 |
| 3:ED:171:GLU:N | 3:ED:171:GLU:OE1 | 2.43 | 0.51 |
| 3:ED:44:SER:HB3 | 3:ED:76:MET:SD | 2.50 | 0.51 |
| 5:EI:51:THR:HA | 5:EI:69:ALA:HB3 | 1.92 | 0.51 |
| 5:EI:79:ILE:HG13 | 5:EI:108:THR:O | 2.10 | 0.51 |
| 4:F:284:ILE:HD11 | 4:H:205:THR:HG22 | 1.91 | 0.51 |
| 5:FA:490:TRP:NE1 | 5:FA:500:ALA:O | 2.44 | 0.51 |
| 7:FE:480:ARG:HD3 | 7:FF:462:ASN:ND2 | 2.25 | 0.51 |
| 7:FE:511:GLU:HB3 | 7:FE:513:ARG:HH11 | 1.74 | 0.51 |
| 7:FE:54:THR:HG22 | 7:FE:55:LYS:O | 2.10 | 0.51 |
| 7:FE:216:MET:SD | 7:FF:202:GLY:HA3 | 2.50 | 0.51 |
| 7:FF:367:VAL:O | 7:FF:389:ASN:HA | 2.10 | 0.51 |
| 7:FF:406:GLY:O | 7:FF:410:THR:HG23 | 2.10 | 0.51 |
| 1:GE:41:ASN:OD1 | 1:GE:42:GLU:N | 2.38 | 0.51 |
| 1:GE:538:VAL:HG11 | 1:GE:558:PHE:CE1 | 2.45 | 0.51 |
| 2:GF:821:ILE:HG22 | 2:GF:822:ALA:N | 2.25 | 0.51 |
| 2:GF:934:ALA:HB1 | 2:GF:942:ILE:HD12 | 1.91 | 0.51 |
| 3:GG:63:ASP:HB2 | 3:GH:13:THR:HG23 | 1.92 | 0.51 |
| 4:GJ:39:TYR:CD1 | 4:HA:7:LYS:HB2 | 2.46 | 0.51 |
| 5:HB:172:GLN:HG2 | 5:HB:173:GLY:H | 1.75 | 0.51 |
| 5:HB:214:SER:OG | 5:HB:222:LEU:O | 2.22 | 0.51 |
| 5:HB:289:LYS:HE2 | 5:HB:370:HIS:HE1 | 1.74 | 0.51 |
| 5:HB:78:THR:HA | 5:HB:108:THR:HB | 1.90 | 0.51 |
| 5:HD:107:VAL:O | 5:HD:125:GLU:HG3 | 2.09 | 0.51 |
| 6:HE:100:PRO:O | 6:HE:103:SER:OG | 2.18 | 0.51 |
| 7:HH:66:VAL:HG21 | 7:HH:80:THR:HB | 1.91 | 0.51 |
| 7:HI:451:PHE:CE1 | 7:HI:470:GLY:HA2 | 2.46 | 0.51 |
| 12:W:167:GLU:HA | 12:IF:211:HIS:HE1 | 1.74 | 0.51 |
| 12:IF:223:VAL:HA | 12:IF:241:VAL:HA | 1.92 | 0.51 |
| 7:O:315:ILE:HG12 | 7:Q:308:ILE:HD12 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:325:TYR:CD1 | 7:P:330:ARG:HA | 2.41 | 0.51 |
| 10:U:340:SER:O | 10:U:341:THR:HG23 | 2.11 | 0.51 |
| 12:W:224:SER:HB3 | 12:W:240:ASP:OD1 | 2.11 | 0.51 |
| 1:X:361:GLN:OE1 | 1:X:362:THR:N | 2.42 | 0.51 |
| 1:X:510:MET:HE1 | 1:X:623:LEU:HD21 | 1.92 | 0.51 |
| 1:Y:156:ASP:HB3 | 1:Y:160:GLN:O | 2.10 | 0.51 |
| 13:YA:379[B]:PRO:HG2 | 13:YA:429[B]:ARG:CZ | 2.40 | 0.51 |
| 13:YA:428[E]:GLY:HA3 | 13:YC:418[E]:THR:HG21 | 1.92 | 0.51 |
| 13:YA:379[F]:PRO:HG2 | 13:YA:429[F]:ARG:CZ | 2.40 | 0.51 |
| 13:YA:436[F]:ASP:OD2 | 13:YA:437[F]:ASN:N | 2.43 | 0.51 |
| 13:YA:538[A]:VAL:HG11 | 13:YB:534[A]:LEU:HB2 | 1.92 | 0.51 |
| 13:YA:538[B]:VAL:HG11 | 13:YB:534[B]:LEU:HB2 | 1.92 | 0.51 |
| 13:YB:436[F]:ASP:OD2 | 13:YB:437[F]:ASN:N | 2.43 | 0.51 |
| 13:YA:454[B]:LYS:NZ | 13:YB:464[B]:TYR:OH | 2.42 | 0.51 |
| 13:YB:503[E]:THR:O | 13:YC:495[E]:THR:HA | 2.10 | 0.51 |
| 13:YC:116[F]:ASP:OD2 | 13:YC:121[F]:TYR:N | 2.43 | 0.51 |
| 13:YC:66[F]:MET:O | 13:YC:69[F]:ILE:N | 2.43 | 0.51 |
| 14:YD:101[E]:GLY:HA2 | 14:YF:332[E]:GLN:OE1 | 2.10 | 0.51 |
| 14:YD:172[C]:TYR:CE1 | 14:YD:176[C]:VAL:HG21 | 2.45 | 0.51 |
| 14:YD:172[E]:TYR:CE1 | 14:YD:176[E]:VAL:HG21 | 2.45 | 0.51 |
| 14:YD:230[A]:LEU:HB2 | 14:YD:313[A]:ILE:HD11 | 1.91 | 0.51 |
| 14:YD:330[C]:LYS:HE3 | 14:YD:330[C]:LYS:HA | 1.91 | 0.51 |
| 14:YF:230[C]:LEU:HB2 | 14:YF:313[C]:ILE:HD11 | 1.91 | 0.51 |
| 11:V:182:ASN:ND2 | 14:YF:327[C]:ASN:HD22 | 2.08 | 0.51 |
| 2:Z:41:THR:O | 2:Z:50:PRO:HD2 | 2.10 | 0.51 |
| 1:A:145:PHE:CD2 | 1:A:169:GLN:OE1 | 2.63 | 0.51 |
| 5:AC:51:THR:HA | 5:AC:69:ALA:HB3 | 1.92 | 0.51 |
| 5:AC:552:VAL:HG11 | 5:AE:569:TYR:CE2 | 2.45 | 0.51 |
| 5:AD:191:ILE:H | 5:AE:164:ARG:HH21 | 1.59 | 0.51 |
| 5:AD:501:LEU:HB3 | 5:AD:512:PRO:HB2 | 1.91 | 0.51 |
| 7:AJ:160:MET:CE | 7:AJ:165:THR:HB | 2.40 | 0.51 |
| 7:AI:59:PHE:CZ | 7:AJ:55:LYS:HG3 | 2.46 | 0.51 |
| 10:BE:340:SER:O | 10:BE:341:THR:HG23 | 2.11 | 0.51 |
| 1:BI:517:PHE:N | 1:BI:536:TYR:O | 2.43 | 0.51 |
| 1:BI:538:VAL:HG11 | 1:BI:558:PHE:CE1 | 2.45 | 0.51 |
| 2:BJ:41:THR:O | 2:BJ:50:PRO:HD2 | 2.10 | 0.51 |
| 2:BJ:701:TRP:CD2 | 2:BJ:701:TRP:O | 2.63 | 0.51 |
| 4:CD:111:ASN:HD21 | 4:CD:116:ILE:H | 1.56 | 0.51 |
| 5:CF:86:VAL:HG22 | 5:CF:87:ASN:H | 1.76 | 0.51 |
| 5:CG:472:TYR:HA | 5:CH:416:ILE:HG23 | 1.92 | 0.51 |
| 5:CH:204:ASP:OD1 | 5:CH:205:VAL:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:995:ASP:HB2 | 5:CH:7:ILE:HG22 | 1.92 | 0.51 |
| 7:DB:159:ALA:HB1 | 7:DC:159:ALA:HB2 | 1.92 | 0.51 |
| 7:DD:149:GLN:O | 7:DD:153:GLY:HA2 | 2.11 | 0.51 |
| 7:DD:167:GLN:O | 7:DD:171:LYS:HG2 | 2.10 | 0.51 |
| 7:DC:210:ILE:O | 7:DD:210:ILE:HG22 | 2.09 | 0.51 |
| 7:DD:386:ASN:OD1 | 7:DD:389:ASN:N | 2.24 | 0.51 |
| 9:DG:95:VAL:HG22 | 9:DG:106:VAL:HG22 | 1.92 | 0.51 |
| 12:BG:126:TYR:HA | 12:DJ:230:TYR:HD2 | 1.75 | 0.51 |
| 1:EB:192:ILE:HG22 | 1:EB:272:TYR:CD1 | 2.45 | 0.51 |
| 2:EC:788:THR:HG23 | 2:EC:790:THR:N | 2.24 | 0.51 |
| 2:EC:919:TYR:HA | 2:EC:990:MET:HE3 | 1.91 | 0.51 |
| 2:EC:934:ALA:HB1 | 2:EC:942:ILE:HD12 | 1.91 | 0.51 |
| 3:ED:108:ILE:H | 3:ED:108:ILE:HD12 | 1.76 | 0.51 |
| 2:EC:9:THR:HG21 | 3:EE:57:ALA:HB3 | 1.92 | 0.51 |
| 3:EE:95:TRP:CD2 | 3:EE:169:PRO:HB3 | 2.45 | 0.51 |
| 4:EF:103:LEU:HD21 | 4:EH:113:ASN:ND2 | 2.22 | 0.51 |
| 4:EG:218:GLU:OE1 | 4:EH:201:LYS:NZ | 2.34 | 0.51 |
| 5:EI:78:THR:HA | 5:EI:108:THR:HB | 1.90 | 0.51 |
| 5:EI:86:VAL:HG22 | 5:EI:87:ASN:H | 1.76 | 0.51 |
| 5:EJ:410:GLN:HG2 | 5:EJ:443:PHE:O | 2.10 | 0.51 |
| 5:EJ:89:TYR:CD1 | 5:EJ:139:ALA:HA | 2.45 | 0.51 |
| 4:F:204:VAL:HG22 | 4:F:276:VAL:HG22 | 1.92 | 0.51 |
| 5:EJ:247:PHE:HZ | 5:FA:162:VAL:HG21 | 1.76 | 0.51 |
| 5:FA:314:ASN:ND2 | 6:FC:8:ALA:O | 2.44 | 0.51 |
| 6:FD:82:VAL:HB | 6:FD:187:LYS:HB3 | 1.92 | 0.51 |
| 7:FF:220:SER:OG | 7:FF:226:GLY:O | 2.28 | 0.51 |
| 7:FG:145:SER:O | 7:FG:164:LYS:NZ | 2.25 | 0.51 |
| 7:FG:167:GLN:O | 7:FG:171:LYS:HG2 | 2.10 | 0.51 |
| 7:FG:77:THR:CG2 | 7:FG:80:THR:H | 2.23 | 0.51 |
| 11:GB:142:LYS:HB3 | 11:GB:143:TYR:CD2 | 2.45 | 0.51 |
| 12:GC:15:ASP:OD1 | 12:GC:16:PHE:N | 2.44 | 0.51 |
| 1:GD:353:PHE:HD2 | 1:GD:392:ILE:HD13 | 1.76 | 0.51 |
| 1:GE:105:ALA:HB2 | 1:GE:275:THR:HG21 | 1.92 | 0.51 |
| 1:GE:363:PHE:CE1 | 1:GE:373:PHE:HD2 | 2.28 | 0.51 |
| 1:GE:411:PRO:HG2 | 1:GE:413:TYR:HE1 | 1.75 | 0.51 |
| 1:GE:443:LYS:HG2 | 1:GE:471:ALA:HB2 | 1.92 | 0.51 |
| 2:GF:193:MET:N | 2:GF:200:TYR:O | 2.37 | 0.51 |
| 2:GF:572:ASN:HB3 | 2:GF:611:ILE:HG22 | 1.92 | 0.51 |
| 3:GG:44:SER:HB3 | 3:GG:76:MET:SD | 2.50 | 0.51 |
| 5:HB:100:ALA:HB2 | 5:HB:130:PHE:CD1 | 2.45 | 0.51 |
| 5:HB:79:ILE:HG13 | 5:HB:108:THR:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:591:PRO:HA | 5:HD:520:GLY:O | 2.11 | 0.51 |
| 7:HH:171:LYS:O | 7:HH:175:GLN:N | 2.43 | 0.51 |
| 7:HI:511:GLU:HB3 | 7:HI:513:ARG:NH1 | 2.25 | 0.51 |
| 5:I:486:VAL:HG11 | 5:K:590:GLN:HE21 | 1.76 | 0.51 |
| 11:IE:30:ARG:HH12 | 11:IE:192:TYR:HD1 | 1.57 | 0.51 |
| 12:IF:216:PHE:HE1 | 12:IF:218:MET:CE | 2.23 | 0.51 |
| 5:I:446:VAL:HG21 | 5:J:443:PHE:CD2 | 2.46 | 0.51 |
| 5:K:460:TYR:CE2 | 5:K:462:ASN:HB2 | 2.46 | 0.51 |
| 7:O:236:VAL:O | 7:O:253:ARG:NH1 | 2.43 | 0.51 |
| 7:P:511:GLU:HB3 | 7:P:513:ARG:NH1 | 2.25 | 0.51 |
| 7:P:84:ARG:NH1 | 7:P:88:PRO:HB3 | 2.25 | 0.51 |
| 7:Q:149:GLN:O | 7:Q:153:GLY:HA2 | 2.10 | 0.51 |
| 7:Q:232:THR:HG22 | 7:Q:235:GLU:HG3 | 1.92 | 0.51 |
| 11:V:47:THR:OG1 | 9:IC:114:ASP:O | 2.27 | 0.51 |
| 13:YA:367[E]:PRO:HA | 13:YC:315[E]:LEU:HD23 | 1.92 | 0.51 |
| 13:YB:379[E]:PRO:HG2 | 13:YB:429[E]:ARG:CZ | 2.40 | 0.51 |
| 13:YB:379[B]:PRO:HG2 | 13:YB:429[B]:ARG:CZ | 2.41 | 0.51 |
| 13:YB:57[F]:VAL:HG11 | 13:YB:76[F]:PRO:HD3 | 1.92 | 0.51 |
| 14:YE:172[E]:TYR:CE1 | 14:YE:176[E]:VAL:HG21 | 2.45 | 0.51 |
| 14:YE:230[A]:LEU:HB2 | 14:YE:313[A]:ILE:HD11 | 1.91 | 0.51 |
| 14:YE:330[D]:LYS:HE3 | 14:YE:330[D]:LYS:HA | 1.92 | 0.51 |
| 2:Z:120:ASN:CB | 2:Z:155:PRO:HB3 | 2.35 | 0.51 |
| 5:AC:190:ASN:CB | 5:AC:247:PHE:HB2 | 2.41 | 0.51 |
| 5:AE:275:SER:HA | 5:AE:280:ILE:HG22 | 1.92 | 0.51 |
| 5:AC:486:VAL:HG22 | 5:AE:591:PRO:O | 2.11 | 0.51 |
| 7:AI:146:SER:HB3 | 7:AI:148:PRO:HD2 | 1.91 | 0.51 |
| 7:AJ:406:GLY:O | 7:AJ:410:THR:HG23 | 2.10 | 0.51 |
| 7:AJ:47:VAL:HG12 | 7:AJ:48:PRO:N | 2.24 | 0.51 |
| 1:B:155:ARG:NH2 | 1:B:159:ASN:HA | 2.26 | 0.51 |
| 1:B:363:PHE:CE1 | 1:B:373:PHE:HD2 | 2.28 | 0.51 |
| 1:B:378:PRO:HG3 | 1:B:384:LEU:HA | 1.93 | 0.51 |
| 1:B:400:ASN:ND2 | 1:B:406:PRO:HD3 | 2.25 | 0.51 |
| 7:BA:232:THR:HG22 | 7:BA:235:GLU:HG3 | 1.92 | 0.51 |
| 7:BA:255:SER:HB3 | 7:BA:263:VAL:CG1 | 2.40 | 0.51 |
| 8:BC:14:ASP:OD2 | 8:BC:17:ARG:NH2 | 2.33 | 0.51 |
| 10:BE:286:VAL:HG22 | 10:BE:287:VAL:H | 1.73 | 0.51 |
| 1:BI:155:ARG:NH2 | 1:BI:159:ASN:HA | 2.26 | 0.51 |
| 1:BI:187:ILE:HD11 | 1:BI:270:ILE:HD13 | 1.93 | 0.51 |
| 1:BI:192:ILE:HG22 | 1:BI:272:TYR:CD1 | 2.45 | 0.51 |
| 2:BJ:782:VAL:HA | 2:BJ:795:VAL:HG23 | 1.92 | 0.51 |
| 2:C:380:ILE:O | 2:C:401:LYS:HD2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:572:ASN:HB3 | 2:C:611:ILE:HG22 | 1.92 | 0.51 |
| 3:CA:232:GLN:N | 3:CA:232:GLN:OE1 | 2.42 | 0.51 |
| 3:CA:44:SER:HB3 | 3:CA:76:MET:SD | 2.50 | 0.51 |
| 4:CC:204:VAL:HG22 | 4:CC:276:VAL:HG22 | 1.92 | 0.51 |
| 4:CD:131:LYS:HD3 | 4:CD:161:ASN:ND2 | 2.25 | 0.51 |
| 5:CH:257:SER:HB2 | 5:CH:387:ASN:HD22 | 1.76 | 0.51 |
| 8:DE:5:ASP:OD1 | 8:DE:8:ARG:NH1 | 2.43 | 0.51 |
| 1:EA:543:THR:CG2 | 1:EA:552:LYS:H | 2.23 | 0.51 |
| 1:EB:187:ILE:HD11 | 1:EB:270:ILE:HD13 | 1.93 | 0.51 |
| 1:EB:400:ASN:ND2 | 1:EB:406:PRO:HD3 | 2.25 | 0.51 |
| 2:EC:575:PHE:O | 2:EC:607:THR:OG1 | 2.13 | 0.51 |
| 2:EC:969:TYR:HD2 | 2:EC:982:LEU:HD13 | 1.75 | 0.51 |
| 5:EI:323:THR:HB | 5:EI:355:ASP:HB3 | 1.93 | 0.51 |
| 5:EJ:289:LYS:O | 5:EJ:290:SER:OG | 2.25 | 0.51 |
| 5:EJ:89:TYR:CE1 | 5:EJ:139:ALA:HA | 2.45 | 0.51 |
| 6:FC:54:SER:HA | 6:FD:164:GLN:HE22 | 1.75 | 0.51 |
| 7:FE:260:ARG:HA | 7:FG:263:VAL:O | 2.11 | 0.51 |
| 7:FG:29:ILE:HG22 | 7:FG:30:THR:N | 2.18 | 0.51 |
| 12:GC:204:HIS:CB | 12:GC:210:PRO:HA | 2.40 | 0.51 |
| 2:GF:225:PHE:CE1 | 2:GF:294:PHE:HD2 | 2.29 | 0.51 |
| 2:GF:41:THR:O | 2:GF:50:PRO:HD2 | 2.10 | 0.51 |
| 2:GF:934:ALA:HB2 | 2:GF:998:GLY:HA2 | 1.93 | 0.51 |
| 3:GG:261:ALA:O | 3:GG:266:ASN:ND2 | 2.30 | 0.51 |
| 5:HB:262:GLN:HG2 | 5:HB:382:ASN:HD22 | 1.76 | 0.51 |
| 5:HC:89:TYR:CD1 | 5:HC:139:ALA:HA | 2.45 | 0.51 |
| 5:HC:180:VAL:HG13 | 5:HC:181:PHE:N | 2.25 | 0.51 |
| 5:HD:204:ASP:OD1 | 5:HD:205:VAL:N | 2.43 | 0.51 |
| 5:HC:313:PHE:HE1 | 6:HE:8:ALA:HB1 | 1.76 | 0.51 |
| 7:HH:216:MET:SD | 7:HI:202:GLY:HA3 | 2.50 | 0.51 |
| 7:HH:236:VAL:O | 7:HH:253:ARG:NH1 | 2.43 | 0.51 |
| 7:HH:54:THR:HG22 | 7:HH:55:LYS:O | 2.10 | 0.51 |
| 7:HJ:129:PHE:O | 7:HJ:141:VAL:HG11 | 2.11 | 0.51 |
| 7:HJ:375:TYR:CE2 | 7:HJ:390:PRO:HB2 | 2.45 | 0.51 |
| 7:HH:512:THR:O | 7:HJ:514:PRO:HB3 | 2.09 | 0.51 |
| 5:I:172:GLN:HG2 | 5:I:173:GLY:H | 1.75 | 0.51 |
| 5:I:1:MET:N | 5:J:41:ASP:HB3 | 2.26 | 0.51 |
| 5:I:86:VAL:HG22 | 5:I:87:ASN:H | 1.76 | 0.51 |
| 5:K:204:ASP:OD1 | 5:K:205:VAL:N | 2.43 | 0.51 |
| 5:K:290:SER:HB3 | 5:K:371:PHE:H | 1.75 | 0.51 |
| 7:O:476:ASP:OD2 | 7:P:454:HIS:HE1 | 1.94 | 0.51 |
| 1:Y:555:ILE:O | 1:Y:589:TYR:HD1 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:116[C]:ASP:OD2 | 13:YA:121[C]:TYR:N | 2.43 | 0.51 |
| 13:YA:116[D]:ASP:OD2 | 13:YA:121[D]:TYR:N | 2.43 | 0.51 |
| 13:YA:270[C]:ASN:O | 13:YA:274[C]:GLN:N | 2.42 | 0.51 |
| 13:YA:256[F]:ILE:HA | 13:YA:286[F]:VAL:HG21 | 1.92 | 0.51 |
| 13:YA:529[B]:THR:N | 13:YB:520[B]:THR:O | 2.44 | 0.51 |
| 13:YA:538[E]:VAL:HG11 | 13:YB:534[E]:LEU:HB2 | 1.92 | 0.51 |
| 13:YB:13[E]:GLY:O | 13:YB:82[E]:VAL:N | 2.44 | 0.51 |
| 13:YB:284[B]:MET:HE3 | 13:YC:363[B]:PRO:CB | 2.35 | 0.51 |
| 13:YC:109[E]:ASN:HB3 | 13:YC:112[E]:GLU:HB2 | 1.93 | 0.51 |
| 13:YC:116[A]:ASP:OD2 | 13:YC:121[A]:TYR:N | 2.43 | 0.51 |
| 13:YC:179[A]:MET:SD | 13:YC:279[A]:ASN:ND2 | 2.76 | 0.51 |
| 14:YD:172[D]:TYR:CE1 | 14:YD:176[D]:VAL:HG21 | 2.45 | 0.51 |
| 14:YD:293[C]:GLU:N | 14:YD:293[C]:GLU:OE1 | 2.44 | 0.51 |
| 14:YD:330[E]:LYS:HE3 | 14:YD:330[E]:LYS:HA | 1.92 | 0.51 |
| 13:YC:90[D]:TRP:NE1 | 14:YF:175[D]:GLU:OE1 | 2.36 | 0.51 |
| 14:YF:232[E]:TYR:HD2 | 14:YF:233[E]:ASP:OD1 | 1.92 | 0.51 |
| 2:Z:380:ILE:O | 2:Z:401:LYS:HD2 | 2.10 | 0.51 |
| 5:AC:213:GLY:O | 5:AC:221:GLU:HB2 | 2.11 | 0.51 |
| 5:AC:323:THR:HB | 5:AC:355:ASP:HB3 | 1.93 | 0.51 |
| 5:AC:64:TRP:CE2 | 5:AC:82:PRO:HG2 | 2.45 | 0.51 |
| 5:AE:200:LEU:HD23 | 5:AE:210:SER:HA | 1.93 | 0.51 |
| 7:AI:236:VAL:O | 7:AI:253:ARG:NH1 | 2.43 | 0.51 |
| 1:B:192:ILE:HG22 | 1:B:272:TYR:CD1 | 2.45 | 0.51 |
| 1:B:443:LYS:HG2 | 1:B:471:ALA:HB2 | 1.92 | 0.51 |
| 7:BA:29:ILE:HG22 | 7:BA:30:THR:N | 2.18 | 0.51 |
| 7:AI:315:ILE:HG12 | 7:BA:308:ILE:HD12 | 1.93 | 0.51 |
| 7:BA:77:THR:CG2 | 7:BA:80:THR:H | 2.23 | 0.51 |
| 8:BB:36:CYS:HA | 8:BB:73:VAL:HG12 | 1.91 | 0.51 |
| 8:BC:72:THR:HA | 8:BC:154:GLU:HA | 1.92 | 0.51 |
| 10:BE:132:SER:HA | 10:BE:209:TRP:NE1 | 2.25 | 0.51 |
| 12:BG:15:ASP:OD1 | 12:BG:16:PHE:N | 2.44 | 0.51 |
| 12:BG:172:ARG:HA | 12:BG:175:GLN:HB3 | 1.93 | 0.51 |
| 1:BH:145:PHE:CD2 | 1:BH:169:GLN:OE1 | 2.63 | 0.51 |
| 1:BI:348:PHE:CZ | 1:BI:399:TYR:HD2 | 2.28 | 0.51 |
| 1:BI:619:GLN:N | 1:BI:619:GLN:OE1 | 2.35 | 0.51 |
| 2:C:107:ALA:HB2 | 2:C:128:THR:HA | 1.91 | 0.51 |
| 2:C:416:VAL:HG23 | 2:C:417:PHE:N | 2.25 | 0.51 |
| 2:C:901:ASN:OD1 | 3:E:333:THR:OG1 | 2.23 | 0.51 |
| 3:CA:279:LEU:HD12 | 3:CB:232:GLN:HE21 | 1.75 | 0.51 |
| 5:CF:194:LYS:HE3 | 5:CH:198:ASN:HD22 | 1.75 | 0.51 |
| 2:BJ:221:ALA:H | 5:CG:562:SER:CB | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:323:THR:HG21 | 5:CH:354:THR:HG23 | 1.91 | 0.51 |
| 5:CF:486:VAL:HG11 | 5:CH:590:GLN:HE21 | 1.75 | 0.51 |
| 6:DA:82:VAL:HB | 6:DA:187:LYS:HB3 | 1.92 | 0.51 |
| 7:DC:160:MET:CE | 7:DC:165:THR:HB | 2.40 | 0.51 |
| 7:DD:77:THR:CG2 | 7:DD:80:THR:H | 2.23 | 0.51 |
| 9:DG:19:TRP:CZ3 | 9:DG:20:ASN:HB3 | 2.46 | 0.51 |
| 3:E:137:PRO:HG3 | 3:E:185:GLY:HA3 | 1.92 | 0.51 |
| 3:E:92:ARG:HD3 | 3:E:205:ASN:O | 2.11 | 0.51 |
| 1:EA:353:PHE:HD2 | 1:EA:392:ILE:HD13 | 1.76 | 0.51 |
| 1:EB:209:TRP:HB2 | 1:EB:225:TYR:HE1 | 1.74 | 0.51 |
| 1:EB:530:LEU:HD12 | 1:EB:531:GLU:N | 2.26 | 0.51 |
| 2:EC:12:ARG:HG3 | 2:EC:24:ARG:HB2 | 1.92 | 0.51 |
| 2:EC:371:ILE:HG13 | 2:EC:372:CYS:H | 1.76 | 0.51 |
| 2:EC:231:TYR:HE2 | 2:EC:389:ASN:HD21 | 1.58 | 0.51 |
| 3:EE:92:ARG:HD3 | 3:EE:205:ASN:O | 2.11 | 0.51 |
| 4:F:82:GLY:O | 4:H:64:THR:N | 2.36 | 0.51 |
| 5:FA:257:SER:HB2 | 5:FA:387:ASN:HD22 | 1.76 | 0.51 |
| 5:FA:460:TYR:CE2 | 5:FA:462:ASN:HB2 | 2.46 | 0.51 |
| 6:FC:35:VAL:HG13 | 6:FC:58:ASP:HB2 | 1.93 | 0.51 |
| 5:EI:239:GLY:O | 7:FE:2:SER:N | 2.44 | 0.51 |
| 9:FJ:125:GLN:OE1 | 9:FJ:125:GLN:N | 2.43 | 0.51 |
| 12:GC:156:ASP:O | 12:GC:245:TYR:HE2 | 1.94 | 0.51 |
| 12:GC:30:PRO:HG3 | 12:GC:197:ALA:HB2 | 1.92 | 0.51 |
| 1:GD:510:MET:HE1 | 1:GD:623:LEU:HD21 | 1.92 | 0.51 |
| 1:GE:153:ALA:HB2 | 1:GE:163:PRO:HB3 | 1.93 | 0.51 |
| 1:GE:156:ASP:HB3 | 1:GE:160:GLN:O | 2.10 | 0.51 |
| 1:GE:123:ILE:HG12 | 1:GE:161:TYR:OH | 2.11 | 0.51 |
| 2:GF:12:ARG:HG3 | 2:GF:24:ARG:HB2 | 1.92 | 0.51 |
| 2:GF:788:THR:HG23 | 2:GF:790:THR:N | 2.24 | 0.51 |
| 3:GG:171:GLU:OE1 | 3:GG:171:GLU:N | 2.43 | 0.51 |
| 3:GG:193:GLU:O | 3:GG:223:TRP:HA | 2.11 | 0.51 |
| 4:GI:39:TYR:CG | 4:GJ:7:LYS:HD3 | 2.45 | 0.51 |
| 5:HB:190:ASN:CB | 5:HB:247:PHE:HB2 | 2.41 | 0.51 |
| 5:HB:264:ARG:HG3 | 5:HB:379:ASP:O | 2.10 | 0.51 |
| 5:HB:86:VAL:HG22 | 5:HB:87:ASN:H | 1.76 | 0.51 |
| 5:HC:311:VAL:HG22 | 5:HC:320:LEU:HD22 | 1.92 | 0.51 |
| 5:HC:19:LEU:HD13 | 5:HD:19:LEU:HD21 | 1.93 | 0.51 |
| 5:HD:305:ASN:N | 5:HD:305:ASN:OD1 | 2.42 | 0.51 |
| 5:HD:490:TRP:NE1 | 5:HD:500:ALA:O | 2.44 | 0.51 |
| 5:HB:46:ALA:N | 5:HD:65:GLY:O | 2.29 | 0.51 |
| 6:HF:14:LEU:O | 6:HF:16:ASP:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:27:PRO:HA | 7:HH:29:ILE:HD11 | 1.92 | 0.51 |
| 7:HJ:289:GLN:OE1 | 7:HJ:294:GLN:NE2 | 2.40 | 0.51 |
| 7:HH:439:ILE:HG23 | 7:HJ:515:TRP:CZ2 | 2.46 | 0.51 |
| 5:I:72:THR:HG22 | 5:I:77:VAL:HG22 | 1.91 | 0.51 |
| 5:J:89:TYR:CD1 | 5:J:139:ALA:HA | 2.45 | 0.51 |
| 5:J:311:VAL:HG22 | 5:J:320:LEU:HD22 | 1.92 | 0.51 |
| 5:I:486:VAL:HG22 | 5:K:591:PRO:O | 2.11 | 0.51 |
| 5:K:78:THR:HA | 5:K:108:THR:HB | 1.92 | 0.51 |
| 7:O:493:GLU:HA | 7:O:496:ARG:HH21 | 1.76 | 0.51 |
| 7:O:66:VAL:HG21 | 7:O:80:THR:HB | 1.91 | 0.51 |
| 7:P:451:PHE:CE1 | 7:P:470:GLY:HA2 | 2.46 | 0.51 |
| 1:Y:123:ILE:HG12 | 1:Y:161:TYR:OH | 2.11 | 0.51 |
| 1:Y:155:ARG:NH2 | 1:Y:159:ASN:HA | 2.26 | 0.51 |
| 1:Y:363:PHE:CE1 | 1:Y:373:PHE:HD2 | 2.28 | 0.51 |
| 1:Y:433:GLU:O | 1:Y:436:LEU:N | 2.42 | 0.51 |
| 1:Y:517:PHE:N | 1:Y:536:TYR:O | 2.43 | 0.51 |
| 1:Y:582:ASN:HD21 | 1:Y:586:ARG:NH2 | 1.98 | 0.51 |
| 13:YA:109[B]:ASN:HB3 | 13:YA:112[B]:GLU:HB2 | 1.93 | 0.51 |
| 13:YA:13[B]:GLY:O | 13:YA:82[B]:VAL:N | 2.44 | 0.51 |
| 13:YA:428[F]:GLY:HA3 | 13:YC:418[F]:THR:HG21 | 1.93 | 0.51 |
| 13:YA:436[C]:ASP:OD2 | 13:YA:437[C]:ASN:N | 2.43 | 0.51 |
| 13:YA:436[D]:ASP:OD2 | 13:YA:437[D]:ASN:N | 2.44 | 0.51 |
| 13:YA:441[F]:ILE:HG21 | 13:YB:378[F]:GLU:OE2 | 2.10 | 0.51 |
| 13:YA:490[D]:VAL:O | 13:YC:498[D]:VAL:HA | 2.11 | 0.51 |
| 13:YA:441[C]:ILE:HG21 | 13:YB:378[C]:GLU:OE2 | 2.10 | 0.51 |
| 13:YA:529[A]:THR:N | 13:YB:520[A]:THR:O | 2.44 | 0.51 |
| 13:YB:13[B]:GLY:O | 13:YB:82[B]:VAL:N | 2.44 | 0.51 |
| 13:YC:116[C]:ASP:OD2 | 13:YC:121[C]:TYR:N | 2.43 | 0.51 |
| 13:YC:270[E]:ASN:O | 13:YC:274[E]:GLN:N | 2.42 | 0.51 |
| 13:YB:284[A]:MET:HE3 | 13:YC:363[A]:PRO:CB | 2.35 | 0.51 |
| 14:YD:172[F]:TYR:CE1 | 14:YD:176[F]:VAL:HG21 | 2.45 | 0.51 |
| 14:YD:230[C]:LEU:HB2 | 14:YD:313[C]:ILE:HD11 | 1.91 | 0.51 |
| 10:ID:285:LEU:HA | 14:YE:215[D]:GLU:HG3 | 1.91 | 0.51 |
| 14:YF:172[B]:TYR:CE1 | 14:YF:176[B]:VAL:HG21 | 2.45 | 0.51 |
| 10:U:285:LEU:HA | 14:YF:215[C]:GLU:CG | 2.39 | 0.51 |
| 14:YF:278[E]:SER:O | 14:YF:279[E]:ARG:NH1 | 2.43 | 0.51 |
| 15:ZA:67[D]:VAL:HG21 | 15:ZA:96[D]:ILE:HB | 1.92 | 0.51 |
| 1:A:208:ASN:ND2 | 1:A:224:TYR:OH | 2.44 | 0.51 |
| 4:AB:131:LYS:HD3 | 4:AB:161:ASN:ND2 | 2.25 | 0.51 |
| 4:AB:204:VAL:HG22 | 4:AB:276:VAL:HG22 | 1.92 | 0.51 |
| 4:AB:27:GLY:HA2 | 4:AB:30:LYS:HD2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:118:LYS:NZ | 5:AC:145:TYR:O | 2.37 | 0.51 |
| 5:AD:240:ASP:OD1 | 7:BA:4:ASN:ND2 | 2.44 | 0.51 |
| 5:AD:308:SER:HG | 5:AE:258:TYR:HD2 | 1.57 | 0.51 |
| 7:AI:159:ALA:HB1 | 7:AJ:159:ALA:HB2 | 1.93 | 0.51 |
| 7:AI:216:MET:SD | 7:AJ:202:GLY:HA3 | 2.50 | 0.51 |
| 7:AI:265:LEU:O | 7:AJ:257:THR:HA | 2.10 | 0.51 |
| 7:AI:27:PRO:HA | 7:AI:29:ILE:HD11 | 1.92 | 0.51 |
| 7:AI:349:TRP:CZ3 | 7:AJ:342:PRO:HG2 | 2.46 | 0.51 |
| 7:AJ:78:PRO:HB2 | 7:BA:69:GLY:HA2 | 1.93 | 0.51 |
| 1:B:123:ILE:HG12 | 1:B:161:TYR:OH | 2.11 | 0.51 |
| 1:B:209:TRP:CZ3 | 1:B:212:LYS:NZ | 2.69 | 0.51 |
| 1:B:112:LEU:HB3 | 1:B:300:ILE:HG22 | 1.92 | 0.51 |
| 7:BA:20:PRO:HD3 | 7:BA:29:ILE:HG21 | 1.92 | 0.51 |
| 7:BA:289:GLN:OE1 | 7:BA:294:GLN:NE2 | 2.41 | 0.51 |
| 1:BI:209:TRP:CZ3 | 1:BI:212:LYS:NZ | 2.69 | 0.51 |
| 1:BI:400:ASN:ND2 | 1:BI:406:PRO:HD3 | 2.25 | 0.51 |
| 1:BI:424:TYR:OH | 1:BI:657:PRO:HG3 | 2.11 | 0.51 |
| 2:BJ:379:ILE:HG13 | 2:BJ:402:GLY:O | 2.11 | 0.51 |
| 2:C:231:TYR:HE2 | 2:C:389:ASN:HD21 | 1.58 | 0.51 |
| 3:CA:216:LEU:HD23 | 3:CA:236:PHE:HB3 | 1.93 | 0.51 |
| 4:CE:204:VAL:HG22 | 4:CE:276:VAL:HG22 | 1.92 | 0.51 |
| 5:CH:192:ARG:HG3 | 5:CH:245:GLU:HB2 | 1.93 | 0.51 |
| 5:CH:200:LEU:HD23 | 5:CH:210:SER:HA | 1.93 | 0.51 |
| 6:CI:54:SER:O | 6:CJ:164:GLN:NE2 | 2.42 | 0.51 |
| 6:CJ:10:VAL:HG22 | 6:DA:13:ARG:HB2 | 1.93 | 0.51 |
| 6:CJ:147:LYS:O | 6:CJ:157:GLU:N | 2.44 | 0.51 |
| 7:DB:54:THR:HG22 | 7:DB:55:LYS:O | 2.10 | 0.51 |
| 7:DC:367:VAL:O | 7:DC:389:ASN:HA | 2.10 | 0.51 |
| 7:DC:451:PHE:CE1 | 7:DC:470:GLY:HA2 | 2.46 | 0.51 |
| 7:DC:84:ARG:NH1 | 7:DC:88:PRO:HB3 | 2.25 | 0.51 |
| 7:DD:375:TYR:CE2 | 7:DD:390:PRO:HB2 | 2.45 | 0.51 |
| 8:DE:72:THR:HA | 8:DE:154:GLU:HA | 1.92 | 0.51 |
| 8:DF:72:THR:HA | 8:DF:154:GLU:HA | 1.92 | 0.51 |
| 2:EC:486:HIS:HD2 | 3:GG:65:VAL:HG13 | 1.76 | 0.51 |
| 3:EE:40:THR:O | 3:EE:273:SER:N | 2.44 | 0.51 |
| 4:EF:53:GLY:O | 4:EG:7:LYS:HB3 | 2.10 | 0.51 |
| 5:EI:175:THR:O | 5:EI:232:LEU:N | 2.35 | 0.51 |
| 5:EI:320:LEU:HG | 5:EI:357:SER:HB3 | 1.92 | 0.51 |
| 5:EI:361:ASP:OD1 | 5:EI:362:GLU:N | 2.43 | 0.51 |
| 5:EJ:110:VAL:HG22 | 5:EJ:123:PRO:HB3 | 1.92 | 0.51 |
| 4:F:53:GLY:O | 4:G:7:LYS:HB3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:392:THR:OG1 | 5:FA:305:ASN:ND2 | 2.44 | 0.51 |
| 6:FB:54:SER:O | 6:FC:164:GLN:NE2 | 2.43 | 0.51 |
| 7:FE:78:PRO:HB3 | 7:FF:66:VAL:HA | 1.92 | 0.51 |
| 7:FF:160:MET:CE | 7:FF:165:THR:HB | 2.40 | 0.51 |
| 7:FE:479:ASN:O | 7:FF:468:PHE:HB2 | 2.10 | 0.51 |
| 7:FG:129:PHE:O | 7:FG:141:VAL:HG11 | 2.11 | 0.51 |
| 10:GA:313:PRO:HG2 | 10:GA:351:ILE:HG22 | 1.93 | 0.51 |
| 1:GE:378:PRO:HG3 | 1:GE:384:LEU:HA | 1.93 | 0.51 |
| 1:GE:400:ASN:ND2 | 1:GE:406:PRO:HD3 | 2.25 | 0.51 |
| 2:GF:371:ILE:HG13 | 2:GF:372:CYS:H | 1.76 | 0.51 |
| 2:GF:168:ILE:HG12 | 2:GF:578:PHE:CZ | 2.46 | 0.51 |
| 2:GF:581:TYR:HA | 2:GF:605:ARG:HG2 | 1.93 | 0.51 |
| 2:GF:701:TRP:O | 2:GF:701:TRP:CD2 | 2.63 | 0.51 |
| 2:GF:773:GLN:N | 2:GF:837:GLU:O | 2.33 | 0.51 |
| 4:HA:204:VAL:HG22 | 4:HA:276:VAL:HG22 | 1.92 | 0.51 |
| 5:HB:267:ASP:OD1 | 5:HB:285:LEU:HB2 | 2.11 | 0.51 |
| 5:HB:86:VAL:HG13 | 5:HB:87:ASN:N | 2.26 | 0.51 |
| 5:HD:102:TRP:HB2 | 5:HD:129:ARG:O | 2.10 | 0.51 |
| 7:HH:59:PHE:CZ | 7:HI:55:LYS:HG3 | 2.45 | 0.51 |
| 7:HH:480:ARG:NE | 7:HI:465:ARG:HG3 | 2.26 | 0.51 |
| 7:HJ:167:GLN:O | 7:HJ:171:LYS:HG2 | 2.10 | 0.51 |
| 5:I:262:GLN:HG2 | 5:I:382:ASN:HD22 | 1.76 | 0.51 |
| 9:IC:105:ILE:HA | 9:IC:125:GLN:HA | 1.93 | 0.51 |
| 11:IE:73:LEU:HD22 | 11:IE:86:TRP:HH2 | 1.75 | 0.51 |
| 12:IF:172:ARG:HA | 12:IF:175:GLN:HB3 | 1.93 | 0.51 |
| 5:J:202:TYR:OH | 5:J:223:VAL:O | 2.18 | 0.51 |
| 5:J:323:THR:CG2 | 5:J:359:GLU:HB2 | 2.39 | 0.51 |
| 5:K:257:SER:HB2 | 5:K:387:ASN:HD22 | 1.76 | 0.51 |
| 7:O:264:LYS:O | 7:O:279:SER:HA | 2.11 | 0.51 |
| 7:O:336:GLU:O | 7:O:340:THR:N | 2.36 | 0.51 |
| 7:P:466:SER:HB3 | 7:P:468:PHE:CE2 | 2.45 | 0.51 |
| 10:U:132:SER:HA | 10:U:209:TRP:NE1 | 2.25 | 0.51 |
| 10:U:332:LEU:HD21 | 10:U:340:SER:CB | 2.41 | 0.51 |
| 11:V:142:LYS:HB3 | 11:V:143:TYR:CD2 | 2.45 | 0.51 |
| 12:W:204:HIS:CB | 12:W:210:PRO:HA | 2.40 | 0.51 |
| 1:X:208:ASN:ND2 | 1:X:224:TYR:OH | 2.44 | 0.51 |
| 13:YA:57[F]:VAL:HG11 | 13:YA:76[F]:PRO:HD3 | 1.91 | 0.51 |
| 13:YB:13[C]:GLY:O | 13:YB:82[C]:VAL:N | 2.44 | 0.51 |
| 13:YB:436[D]:ASP:OD2 | 13:YB:437[D]:ASN:N | 2.44 | 0.51 |
| 13:YB:503[D]:THR:O | 13:YC:495[D]:THR:HA | 2.10 | 0.51 |
| 13:YB:82[F]:VAL:HG22 | 13:YB:98[F]:GLY:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:116[D]:ASP:OD2 | 13:YC:121[D]:TYR:N | 2.43 | 0.51 |
| 13:YC:13[E]:GLY:O | 13:YC:82[E]:VAL:N | 2.44 | 0.51 |
| 13:YA:407[B]:PRO:HB3 | 13:YC:232[B]:ASN:HB3 | 1.93 | 0.51 |
| 13:YC:436[A]:ASP:OD2 | 13:YC:437[A]:ASN:N | 2.44 | 0.51 |
| 13:YA:76[C]:PRO:CA | 13:YC:61[C]:ILE:HA | 2.41 | 0.51 |
| 13:YC:13[C]:GLY:O | 13:YC:82[C]:VAL:N | 2.44 | 0.51 |
| 14:YD:278[B]:SER:O | 14:YD:279[B]:ARG:NH1 | 2.42 | 0.51 |
| 14:YD:332[A]:GLN:OE1 | 14:YE:101[A]:GLY:HA2 | 2.11 | 0.51 |
| 14:YE:360[C]:ASN:ND2 | 14:YE:360[C]:ASN:H | 2.04 | 0.51 |
| 14:YF:172[C]:TYR:CE1 | 14:YF:176[C]:VAL:HG21 | 2.45 | 0.51 |
| 14:YF:330[F]:LYS:HA | 14:YF:330[F]:LYS:HE3 | 1.91 | 0.51 |
| 1:BH:287:SER:HB2 | 14:YF:373[F]:LYS:HD2 | 1.93 | 0.51 |
| 1:A:559:ALA:HB3 | 1:A:562:ASP:OD2 | 2.11 | 0.51 |
| 1:A:627:PRO:HG3 | 1:A:632:ILE:HD11 | 1.92 | 0.51 |
| 5:AC:100:ALA:HB2 | 5:AC:130:PHE:CD1 | 2.45 | 0.51 |
| 5:AE:257:SER:HB2 | 5:AE:387:ASN:HD22 | 1.76 | 0.51 |
| 6:AF:35:VAL:HG13 | 6:AF:58:ASP:HB2 | 1.93 | 0.51 |
| 6:AF:15:ALA:HB2 | 6:AH:52:ILE:HD11 | 1.92 | 0.51 |
| 7:AI:211:SER:O | 7:AI:215:PHE:N | 2.43 | 0.51 |
| 7:AJ:476:ASP:OD1 | 7:AJ:479:ASN:ND2 | 2.40 | 0.51 |
| 7:AI:202:GLY:HA3 | 7:BA:216:MET:SD | 2.51 | 0.51 |
| 8:BB:72:THR:HA | 8:BB:154:GLU:HA | 1.92 | 0.51 |
| 11:BF:31:ASN:OD1 | 11:BF:32:TYR:N | 2.41 | 0.51 |
| 1:BI:104:SER:OG | 1:BI:316:GLY:O | 2.18 | 0.51 |
| 1:BI:530:LEU:HD12 | 1:BI:531:GLU:N | 2.26 | 0.51 |
| 2:BJ:233:LEU:HD23 | 2:BJ:234:SER:OG | 2.10 | 0.51 |
| 2:BJ:258:LYS:HG2 | 2:BJ:292:GLU:HG3 | 1.92 | 0.51 |
| 2:BJ:664:PHE:HB2 | 9:DG:15:MET:CB | 2.40 | 0.51 |
| 2:C:193:MET:HG3 | 2:C:238:TYR:CZ | 2.46 | 0.51 |
| 2:C:316:ASP:HA | 2:C:331:THR:O | 2.11 | 0.51 |
| 2:C:106:ASN:ND2 | 2:C:626:GLN:HB2 | 2.26 | 0.51 |
| 2:C:726:PHE:O | 2:C:729:SER:OG | 2.16 | 0.51 |
| 2:C:853:ASP:HB2 | 2:C:855:ILE:HG22 | 1.92 | 0.51 |
| 3:CA:108:ILE:H | 3:CA:108:ILE:HD12 | 1.76 | 0.51 |
| 3:CA:171:GLU:N | 3:CA:171:GLU:OE1 | 2.43 | 0.51 |
| 4:CC:61:ILE:O | 4:CD:4:GLN:NE2 | 2.42 | 0.51 |
| 5:CF:172:GLN:HG2 | 5:CF:173:GLY:H | 1.75 | 0.51 |
| 5:CF:190:ASN:CB | 5:CF:247:PHE:HB2 | 2.41 | 0.51 |
| 5:CF:64:TRP:O | 5:CF:93:ILE:HG22 | 2.10 | 0.51 |
| 6:CJ:35:VAL:HG13 | 6:CJ:58:ASP:HB2 | 1.93 | 0.51 |
| 6:DA:147:LYS:O | 6:DA:157:GLU:N | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:163:LEU:O | 7:DB:167:GLN:N | 2.25 | 0.51 |
| 11:DI:73:LEU:HD22 | 11:DI:86:TRP:HH2 | 1.75 | 0.51 |
| 2:EC:379:ILE:HG13 | 2:EC:402:GLY:O | 2.10 | 0.51 |
| 2:EC:934:ALA:HB2 | 2:EC:998:GLY:HA2 | 1.93 | 0.51 |
| 3:EE:232:GLN:O | 3:EE:232:GLN:HG2 | 2.10 | 0.51 |
| 5:EI:268:SER:N | 5:EI:283:THR:O | 2.35 | 0.51 |
| 4:F:27:GLY:HA2 | 4:F:30:LYS:HD2 | 1.91 | 0.51 |
| 6:FC:82:VAL:HB | 6:FC:187:LYS:HB3 | 1.92 | 0.51 |
| 7:FE:45:ASN:CG | 7:FF:24:ASN:HD21 | 2.14 | 0.51 |
| 7:FF:518:SER:HB3 | 7:FG:403:SER:HA | 1.92 | 0.51 |
| 7:FE:512:THR:O | 7:FG:514:PRO:HB3 | 2.11 | 0.51 |
| 4:G:131:LYS:HD3 | 4:G:161:ASN:ND2 | 2.25 | 0.51 |
| 4:G:39:TYR:CD1 | 4:H:7:LYS:HB2 | 2.46 | 0.51 |
| 12:GC:172:ARG:HA | 12:GC:175:GLN:HB3 | 1.93 | 0.51 |
| 1:GD:543:THR:CG2 | 1:GD:552:LYS:H | 2.23 | 0.51 |
| 2:GF:408:HIS:HB3 | 2:GF:410:GLU:CD | 2.31 | 0.51 |
| 4:GJ:204:VAL:HG22 | 4:GJ:276:VAL:HG22 | 1.92 | 0.51 |
| 5:HB:323:THR:HB | 5:HB:355:ASP:HB3 | 1.93 | 0.51 |
| 5:HB:361:ASP:OD1 | 5:HB:362:GLU:N | 2.43 | 0.51 |
| 5:HC:291:ILE:HG22 | 5:HC:292:PRO:O | 2.10 | 0.51 |
| 5:HD:194:LYS:O | 5:HD:242:VAL:HA | 2.11 | 0.51 |
| 5:HD:261:ARG:HD2 | 5:HD:297:GLY:HA3 | 1.92 | 0.51 |
| 6:HE:82:VAL:HB | 6:HE:187:LYS:HB3 | 1.92 | 0.51 |
| 6:HG:147:LYS:O | 6:HG:157:GLU:N | 2.44 | 0.51 |
| 6:HG:82:VAL:HB | 6:HG:187:LYS:HB3 | 1.92 | 0.51 |
| 7:HH:493:GLU:HA | 7:HH:496:ARG:HH21 | 1.76 | 0.51 |
| 7:HJ:20:PRO:HD3 | 7:HJ:29:ILE:HG21 | 1.92 | 0.51 |
| 7:HH:346:ILE:N | 7:HJ:348:MET:O | 2.28 | 0.51 |
| 5:I:213:GLY:O | 5:I:221:GLU:HB2 | 2.11 | 0.51 |
| 10:ID:286:VAL:HG13 | 14:YE:100[F]:LYS:HE2 | 1.93 | 0.51 |
| 10:ID:329:PHE:O | 10:ID:330:ASN:ND2 | 2.44 | 0.51 |
| 10:ID:340:SER:O | 10:ID:341:THR:HG23 | 2.11 | 0.51 |
| 5:K:490:TRP:NE1 | 5:K:500:ALA:O | 2.44 | 0.51 |
| 5:K:356:TYR:CE1 | 6:M:4:LEU:HD13 | 2.45 | 0.51 |
| 6:M:32:ARG:NH1 | 6:N:144:ASN:OD1 | 2.42 | 0.51 |
| 7:O:349:TRP:CZ3 | 7:P:342:PRO:HG2 | 2.45 | 0.51 |
| 7:O:511:GLU:HB3 | 7:O:513:ARG:HH11 | 1.74 | 0.51 |
| 7:P:239:ASN:OD1 | 7:P:253:ARG:NH2 | 2.40 | 0.51 |
| 7:Q:129:PHE:O | 7:Q:141:VAL:HG11 | 2.11 | 0.51 |
| 10:U:313:PRO:HG2 | 10:U:351:ILE:HG22 | 1.93 | 0.51 |
| 13:YA:179[B]:MET:SD | 13:YA:279[B]:ASN:ND2 | 2.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:538[C]:VAL:HG11 | 13:YB:534[C]:LEU:HB2 | 1.92 | 0.51 |
| 13:YB:379[C]:PRO:HG2 | 13:YB:429[C]:ARG:CZ | 2.40 | 0.51 |
| 13:YA:538[F]:VAL:HG11 | 13:YB:534[F]:LEU:HB2 | 1.92 | 0.51 |
| 13:YC:379[B]:PRO:HG2 | 13:YC:429[B]:ARG:CZ | 2.40 | 0.51 |
| 13:YB:571[D]:ARG:HB3 | 13:YC:564[D]:GLN:NE2 | 2.26 | 0.51 |
| 13:YC:82[F]:VAL:HG22 | 13:YC:98[F]:GLY:O | 2.10 | 0.51 |
| 14:YD:124[B]:PHE:CE2 | 14:YD:135[B]:MET:HE2 | 2.45 | 0.51 |
| 14:YD:232[C]:TYR:HD2 | 14:YD:233[C]:ASP:OD1 | 1.92 | 0.51 |
| 14:YD:278[E]:SER:O | 14:YD:279[E]:ARG:NH1 | 2.42 | 0.51 |
| 14:YE:124[D]:PHE:CE2 | 14:YE:135[D]:MET:HE2 | 2.46 | 0.51 |
| 14:YE:124[F]:PHE:CE2 | 14:YE:135[F]:MET:HE2 | 2.45 | 0.51 |
| 14:YE:124[E]:PHE:CE2 | 14:YE:135[E]:MET:HE2 | 2.46 | 0.51 |
| 14:YF:172[D]:TYR:CE1 | 14:YF:176[D]:VAL:HG21 | 2.46 | 0.51 |
| 2:Z:106:ASN:ND2 | 2:Z:626:GLN:HB2 | 2.26 | 0.51 |
| 2:Z:193:MET:HG3 | 2:Z:238:TYR:CZ | 2.46 | 0.51 |
| 5:AD:89:TYR:CE1 | 5:AD:139:ALA:HA | 2.45 | 0.51 |
| 5:AD:410:GLN:HG2 | 5:AD:443:PHE:O | 2.10 | 0.51 |
| 5:AE:285:LEU:HD21 | 5:AE:375:PHE:H | 1.76 | 0.51 |
| 6:AG:14:LEU:O | 6:AG:16:ASP:N | 2.43 | 0.51 |
| 6:AG:35:VAL:HG13 | 6:AG:58:ASP:HB2 | 1.93 | 0.51 |
| 7:AI:99:ARG:NH1 | 7:AI:105:GLU:OE2 | 2.32 | 0.51 |
| 7:AI:145:SER:O | 7:AI:164:LYS:HE2 | 2.11 | 0.51 |
| 7:AI:171:LYS:O | 7:AI:175:GLN:N | 2.43 | 0.51 |
| 7:AJ:399:PHE:HZ | 7:AJ:516:ASN:HD22 | 1.58 | 0.51 |
| 7:AI:452:GLY:HA3 | 7:BA:480:ARG:O | 2.10 | 0.51 |
| 10:BE:323:LYS:HB3 | 10:BE:339:PRO:HG3 | 1.92 | 0.51 |
| 12:BG:156:ASP:O | 12:BG:245:TYR:HE2 | 1.94 | 0.51 |
| 1:BH:460:ALA:HA | 1:BH:631:VAL:HG12 | 1.93 | 0.51 |
| 2:BJ:103:PHE:CZ | 2:BJ:626:GLN:O | 2.64 | 0.51 |
| 2:BJ:646:ARG:CD | 2:BJ:673:GLN:HE22 | 2.13 | 0.51 |
| 2:BJ:773:GLN:N | 2:BJ:837:GLU:O | 2.33 | 0.51 |
| 2:C:1005:ARG:HG3 | 5:I:12:ASP:OD2 | 2.11 | 0.51 |
| 2:C:233:LEU:HD23 | 2:C:234:SER:OG | 2.10 | 0.51 |
| 2:C:408:HIS:HB3 | 2:C:410:GLU:CD | 2.31 | 0.51 |
| 4:CC:172:GLU:HA | 4:CD:166:SER:H | 1.74 | 0.51 |
| 5:CF:267:ASP:OD1 | 5:CF:285:LEU:HB2 | 2.11 | 0.51 |
| 5:CG:180:VAL:HG13 | 5:CG:181:PHE:N | 2.25 | 0.51 |
| 5:CF:200:LEU:HD11 | 5:CG:241:THR:HG21 | 1.93 | 0.51 |
| 5:CH:490:TRP:NE1 | 5:CH:500:ALA:O | 2.44 | 0.51 |
| 7:DB:154:ALA:HB3 | 7:DD:162:PRO:HG2 | 1.93 | 0.51 |
| 7:DB:47:VAL:HG12 | 7:DB:48:PRO:N | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:DJ:156:ASP:O | 12:DJ:245:TYR:HE2 | 1.94 | 0.51 |
| 12:DJ:172:ARG:HA | 12:DJ:175:GLN:HB3 | 1.93 | 0.51 |
| 12:DJ:204:HIS:CB | 12:DJ:210:PRO:HA | 2.40 | 0.51 |
| 1:EA:145:PHE:CD2 | 1:EA:169:GLN:OE1 | 2.63 | 0.51 |
| 1:EA:400:ASN:O | 1:EB:341:THR:HA | 2.11 | 0.51 |
| 1:EB:155:ARG:NH2 | 1:EB:159:ASN:HA | 2.26 | 0.51 |
| 1:EB:227:ARG:HB2 | 1:EB:237:TYR:HE2 | 1.76 | 0.51 |
| 2:EC:41:THR:O | 2:EC:50:PRO:HD2 | 2.10 | 0.51 |
| 3:ED:279:LEU:HD12 | 3:EE:232:GLN:HE21 | 1.75 | 0.51 |
| 5:EI:213:GLY:O | 5:EI:221:GLU:HB2 | 2.11 | 0.51 |
| 5:EI:267:ASP:OD1 | 5:EI:285:LEU:HB2 | 2.11 | 0.51 |
| 5:EI:577:ASN:ND2 | 5:EJ:529:ASN:OD1 | 2.29 | 0.51 |
| 5:EI:569:TYR:CE2 | 5:FA:542:LEU:HD11 | 2.46 | 0.51 |
| 5:FA:78:THR:HA | 5:FA:108:THR:HB | 1.92 | 0.51 |
| 6:FD:35:VAL:HG13 | 6:FD:58:ASP:HB2 | 1.93 | 0.51 |
| 5:EI:318:GLN:NE2 | 6:FD:7:LYS:HB3 | 2.26 | 0.51 |
| 7:FE:171:LYS:O | 7:FE:175:GLN:N | 2.43 | 0.51 |
| 7:FE:236:VAL:O | 7:FE:253:ARG:NH1 | 2.44 | 0.51 |
| 7:FE:47:VAL:HG12 | 7:FE:48:PRO:N | 2.26 | 0.51 |
| 7:FE:72:ASN:HA | 7:FG:77:THR:HG21 | 1.92 | 0.51 |
| 10:GA:323:LYS:HB3 | 10:GA:339:PRO:HG3 | 1.92 | 0.51 |
| 1:GD:287:SER:HB2 | 14:YD:373[F]:LYS:HD2 | 1.93 | 0.51 |
| 1:GD:560:SER:HA | 1:GD:588:LYS:HD3 | 1.92 | 0.51 |
| 2:GF:258:LYS:HG2 | 2:GF:292:GLU:HG3 | 1.92 | 0.51 |
| 2:GF:816:LEU:HB2 | 3:GH:201:ASN:HD22 | 1.76 | 0.51 |
| 4:HA:27:GLY:HA2 | 4:HA:30:LYS:HD2 | 1.91 | 0.51 |
| 5:HB:94:ARG:HD3 | 5:HB:134:GLU:HG2 | 1.93 | 0.51 |
| 5:HB:213:GLY:O | 5:HB:221:GLU:HB2 | 2.11 | 0.51 |
| 5:HB:45:SER:OG | 5:HD:66:LYS:HA | 2.11 | 0.51 |
| 5:HD:275:SER:HA | 5:HD:280:ILE:HG22 | 1.92 | 0.51 |
| 5:HC:542:LEU:HD21 | 5:HD:569:TYR:OH | 2.11 | 0.51 |
| 6:HF:29:VAL:O | 6:HF:32:ARG:N | 2.36 | 0.51 |
| 7:HH:264:LYS:O | 7:HH:279:SER:HA | 2.11 | 0.51 |
| 7:HJ:149:GLN:O | 7:HJ:153:GLY:HA2 | 2.10 | 0.51 |
| 11:IE:178:ASN:H | 14:YD:217[F]:SER:C | 2.14 | 0.51 |
| 5:K:72:THR:HG22 | 5:K:77:VAL:HG22 | 1.92 | 0.51 |
| 5:J:356:TYR:CE1 | 6:L:4:LEU:HD13 | 2.45 | 0.51 |
| 7:O:146:SER:HB3 | 7:O:148:PRO:HD2 | 1.91 | 0.51 |
| 7:O:171:LYS:O | 7:O:175:GLN:N | 2.43 | 0.51 |
| 7:O:452:GLY:HA3 | 7:Q:480:ARG:O | 2.11 | 0.51 |
| 12:W:230:TYR:HD2 | 12:IF:126:TYR:HA | 1.73 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:444:ILE:O | 1:X:447:TYR:N | 2.43 | 0.51 |
| 1:Y:105:ALA:HB2 | 1:Y:275:THR:HG21 | 1.92 | 0.51 |
| 1:Y:547:SER:O | 1:Y:548:LYS:HG2 | 2.10 | 0.51 |
| 1:Y:538:VAL:HG11 | 1:Y:558:PHE:CE1 | 2.45 | 0.51 |
| 13:YA:13[C]:GLY:O | 13:YA:82[C]:VAL:N | 2.44 | 0.51 |
| 13:YA:66[C]:MET:O | 13:YA:69[C]:ILE:N | 2.44 | 0.51 |
| 13:YA:538[D]:VAL:HG11 | 13:YB:534[D]:LEU:HB2 | 1.92 | 0.51 |
| 13:YB:71[B]:GLY:HA2 | 13:YC:393[B]:MET:HA | 1.93 | 0.51 |
| 13:YB:503[A]:THR:O | 13:YC:495[A]:THR:HA | 2.10 | 0.51 |
| 13:YB:571[E]:ARG:HB3 | 13:YC:564[E]:GLN:NE2 | 2.26 | 0.51 |
| 14:YE:232[A]:TYR:HD2 | 14:YE:233[A]:ASP:OD1 | 1.92 | 0.51 |
| 13:YB:24[C]:LEU:HD23 | 14:YE:259[C]:LEU:HD22 | 1.93 | 0.51 |
| 13:YB:24[F]:LEU:HD23 | 14:YE:259[F]:LEU:HD22 | 1.92 | 0.51 |
| 14:YF:124[C]:PHE:CE2 | 14:YF:135[C]:MET:HE2 | 2.46 | 0.51 |
| 2:Z:701:TRP:O | 2:Z:701:TRP:CD2 | 2.63 | 0.51 |
| 15:ZA:67[B]:VAL:HG21 | 15:ZA:96[B]:ILE:HB | 1.92 | 0.51 |
| 15:ZA:67[F]:VAL:HG21 | 15:ZA:96[F]:ILE:HB | 1.92 | 0.51 |
| 1:A:460:ALA:HA | 1:A:631:VAL:HG12 | 1.93 | 0.51 |
| 5:AC:267:ASP:OD1 | 5:AC:285:LEU:HB2 | 2.11 | 0.51 |
| 5:AE:72:THR:HG22 | 5:AE:77:VAL:HG22 | 1.92 | 0.51 |
| 6:AG:82:VAL:HB | 6:AG:187:LYS:HB3 | 1.92 | 0.51 |
| 6:AH:149:HIS:HB3 | 6:AH:152:ASP:O | 2.11 | 0.51 |
| 6:AH:29:VAL:O | 6:AH:32:ARG:N | 2.36 | 0.51 |
| 7:AI:493:GLU:HA | 7:AI:496:ARG:HH21 | 1.76 | 0.51 |
| 7:AJ:340:THR:HG22 | 7:AJ:341:ILE:HG12 | 1.93 | 0.51 |
| 1:B:530:LEU:HD12 | 1:B:531:GLU:N | 2.26 | 0.51 |
| 7:BA:129:PHE:O | 7:BA:141:VAL:HG11 | 2.11 | 0.51 |
| 9:BD:95:VAL:HG22 | 9:BD:106:VAL:HG22 | 1.92 | 0.51 |
| 11:BF:142:LYS:HB3 | 11:BF:143:TYR:CD2 | 2.45 | 0.51 |
| 1:BH:344:ASP:O | 1:BH:347:THR:N | 2.44 | 0.51 |
| 1:BH:444:ILE:O | 1:BH:447:TYR:N | 2.43 | 0.51 |
| 1:BH:543:THR:CG2 | 1:BH:552:LYS:H | 2.23 | 0.51 |
| 2:C:168:ILE:HG12 | 2:C:578:PHE:CZ | 2.46 | 0.51 |
| 2:C:575:PHE:O | 2:C:607:THR:OG1 | 2.13 | 0.51 |
| 3:CB:95:TRP:CD2 | 3:CB:169:PRO:HB3 | 2.45 | 0.51 |
| 4:CD:39:TYR:CD1 | 4:CE:7:LYS:HB2 | 2.46 | 0.51 |
| 5:CF:213:GLY:O | 5:CF:221:GLU:HB2 | 2.11 | 0.51 |
| 5:CF:323:THR:HB | 5:CF:355:ASP:HB3 | 1.93 | 0.51 |
| 5:CF:20:ARG:CZ | 5:CH:7:ILE:HD12 | 2.41 | 0.51 |
| 6:CI:73:ASN:HD21 | 6:CI:215:PHE:HE2 | 1.59 | 0.51 |
| 6:CJ:14:LEU:O | 6:CJ:16:ASP:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:236:VAL:O | 7:DB:253:ARG:NH1 | 2.44 | 0.51 |
| 7:DB:264:LYS:O | 7:DB:279:SER:HA | 2.11 | 0.51 |
| 7:DB:49:ASP:O | 7:DB:56:GLY:HA3 | 2.09 | 0.51 |
| 7:DB:439:ILE:HG23 | 7:DD:515:TRP:CZ2 | 2.45 | 0.51 |
| 1:EA:80:MET:HE3 | 1:EA:326:ARG:HA | 1.92 | 0.51 |
| 1:EB:153:ALA:HB2 | 1:EB:163:PRO:HB3 | 1.93 | 0.51 |
| 1:EB:424:TYR:OH | 1:EB:657:PRO:HG3 | 2.11 | 0.51 |
| 2:EC:106:ASN:ND2 | 2:EC:626:GLN:HB2 | 2.26 | 0.51 |
| 2:EC:193:MET:HG3 | 2:EC:238:TYR:CZ | 2.46 | 0.51 |
| 2:EC:233:LEU:HD23 | 2:EC:234:SER:OG | 2.10 | 0.51 |
| 2:EC:581:TYR:HA | 2:EC:605:ARG:HG2 | 1.93 | 0.51 |
| 5:EI:86:VAL:HG13 | 5:EI:87:ASN:N | 2.26 | 0.51 |
| 5:EJ:339:GLU:HB3 | 6:FD:172:SER:O | 2.10 | 0.51 |
| 5:FA:180:VAL:HG13 | 5:FA:181:PHE:N | 2.26 | 0.51 |
| 5:FA:275:SER:HA | 5:FA:280:ILE:HG22 | 1.92 | 0.51 |
| 6:FB:149:HIS:HB3 | 6:FB:152:ASP:O | 2.11 | 0.51 |
| 7:FE:90:ALA:HB2 | 7:FE:96:GLY:CA | 2.42 | 0.51 |
| 7:FF:340:THR:HG22 | 7:FF:341:ILE:HG12 | 1.93 | 0.51 |
| 7:FF:447:HIS:CD2 | 7:FG:447:HIS:CD2 | 2.99 | 0.51 |
| 1:EA:52:ARG:HD3 | 9:FJ:22:ASP:OD2 | 2.10 | 0.51 |
| 4:G:218:GLU:OE1 | 4:H:201:LYS:NZ | 2.37 | 0.51 |
| 1:GE:530:LEU:HD12 | 1:GE:531:GLU:N | 2.26 | 0.51 |
| 2:GF:644:ASP:O | 11:IE:84:TYR:OH | 2.28 | 0.51 |
| 4:GI:284:ILE:HD11 | 4:HA:205:THR:HG22 | 1.93 | 0.51 |
| 5:HB:20:ARG:CZ | 5:HD:7:ILE:HD12 | 2.41 | 0.51 |
| 5:HD:460:TYR:CE2 | 5:HD:462:ASN:HB2 | 2.46 | 0.51 |
| 5:HC:356:TYR:CE1 | 6:HE:4:LEU:HD13 | 2.45 | 0.51 |
| 6:HF:35:VAL:HG13 | 6:HF:58:ASP:HB2 | 1.93 | 0.51 |
| 6:HG:35:VAL:HG13 | 6:HG:58:ASP:HB2 | 1.93 | 0.51 |
| 5:I:190:ASN:CB | 5:I:247:PHE:HB2 | 2.41 | 0.51 |
| 5:I:86:VAL:HG13 | 5:I:87:ASN:N | 2.26 | 0.51 |
| 5:I:255:ARG:NH2 | 5:K:390:LEU:HB2 | 2.25 | 0.51 |
| 5:J:472:TYR:HA | 5:K:416:ILE:HG23 | 1.92 | 0.51 |
| 6:N:147:LYS:O | 6:N:157:GLU:N | 2.44 | 0.51 |
| 7:O:509:GLY:HA3 | 7:P:441:GLN:NE2 | 2.26 | 0.51 |
| 1:Y:153:ALA:HB2 | 1:Y:163:PRO:HB3 | 1.93 | 0.51 |
| 1:Y:443:LYS:HG2 | 1:Y:471:ALA:HB2 | 1.92 | 0.51 |
| 1:Y:530:LEU:HD12 | 1:Y:531:GLU:N | 2.26 | 0.51 |
| 13:YA:179[C]:MET:SD | 13:YA:279[C]:ASN:ND2 | 2.75 | 0.51 |
| 13:YA:379[A]:PRO:HG2 | 13:YA:429[A]:ARG:CZ | 2.41 | 0.51 |
| 13:YA:430[B]:ARG:HB3 | 13:YC:434[B]:THR:HG21 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:109[B]:ASN:HB3 | 13:YB:112[B]:GLU:HB2 | 1.93 | 0.51 |
| 13:YB:344[D]:LYS:HA | 13:YB:344[D]:LYS:HE2 | 1.93 | 0.51 |
| 13:YC:379[D]:PRO:HG2 | 13:YC:429[D]:ARG:CZ | 2.41 | 0.51 |
| 13:YC:436[C]:ASP:OD2 | 13:YC:437[C]:ASN:N | 2.43 | 0.51 |
| 13:YC:436[D]:ASP:OD2 | 13:YC:437[D]:ASN:N | 2.44 | 0.51 |
| 13:YB:503[B]:THR:O | 13:YC:495[B]:THR:HA | 2.10 | 0.51 |
| 13:YB:503[F]:THR:O | 13:YC:495[F]:THR:HA | 2.10 | 0.51 |
| 13:YB:571[D]:ARG:HD3 | 13:YC:564[D]:GLN:HE22 | 1.77 | 0.51 |
| 1:EA:130:ARG:HD3 | 14:YD:181[E]:GLY:HA2 | 1.91 | 0.51 |
| 14:YD:360[E]:ASN:H | 14:YD:360[E]:ASN:ND2 | 2.04 | 0.51 |
| 14:YF:330[E]:LYS:HA | 14:YF:330[E]:LYS:HE3 | 1.92 | 0.51 |
| 14:YF:373[D]:LYS:HG2 | 14:YF:374[D]:ASN:N | 2.26 | 0.51 |
| 15:ZA:76[A]:GLN:HB3 | 15:ZA:96[A]:ILE:HD11 | 1.92 | 0.51 |
| 1:A:539:ARG:CD | 1:A:580:LEU:HD23 | 2.42 | 0.50 |
| 5:AC:194:LYS:HB2 | 5:AC:243:GLN:HB2 | 1.92 | 0.50 |
| 5:AD:311:VAL:HG22 | 5:AD:320:LEU:HD22 | 1.92 | 0.50 |
| 5:AD:357:SER:OG | 6:AF:4:LEU:HD21 | 2.10 | 0.50 |
| 5:AE:356:TYR:CE1 | 6:AG:4:LEU:HD13 | 2.46 | 0.50 |
| 6:AF:204:ASP:OD1 | 6:AH:200:THR:N | 2.39 | 0.50 |
| 6:AH:82:VAL:HB | 6:AH:187:LYS:HB3 | 1.92 | 0.50 |
| 7:AI:485:ASN:C | 7:AJ:446:LYS:HG2 | 2.32 | 0.50 |
| 7:AI:72:ASN:HA | 7:BA:77:THR:HG21 | 1.92 | 0.50 |
| 9:BD:19:TRP:CZ3 | 9:BD:20:ASN:HB3 | 2.46 | 0.50 |
| 1:BH:361:GLN:OE1 | 1:BH:362:THR:N | 2.42 | 0.50 |
| 1:BI:123:ILE:HG12 | 1:BI:161:TYR:OH | 2.11 | 0.50 |
| 1:BI:348:PHE:CZ | 1:BI:399:TYR:CD2 | 2.99 | 0.50 |
| 2:BJ:17:SER:HA | 2:BJ:106:ASN:HB3 | 1.93 | 0.50 |
| 2:BJ:225:PHE:CE1 | 2:BJ:294:PHE:HD2 | 2.29 | 0.50 |
| 2:BJ:581:TYR:HA | 2:BJ:605:ARG:HG2 | 1.93 | 0.50 |
| 2:C:225:PHE:CE1 | 2:C:294:PHE:HD2 | 2.28 | 0.50 |
| 2:C:934:ALA:HB2 | 2:C:998:GLY:HA2 | 1.93 | 0.50 |
| 3:CB:40:THR:O | 3:CB:273:SER:N | 2.44 | 0.50 |
| 4:CD:30:LYS:O | 4:CD:34:ASP:N | 2.45 | 0.50 |
| 5:CF:320:LEU:HG | 5:CF:357:SER:HB3 | 1.92 | 0.50 |
| 5:CF:423:THR:O | 7:HJ:495:GLN:NE2 | 2.30 | 0.50 |
| 5:CF:86:VAL:HG13 | 5:CF:87:ASN:N | 2.26 | 0.50 |
| 5:CG:415:ASP:HB2 | 5:CG:440:GLN:HE22 | 1.76 | 0.50 |
| 5:CH:261:ARG:HD2 | 5:CH:297:GLY:HA3 | 1.92 | 0.50 |
| 5:CH:397:ASP:O | 5:CH:400:ILE:HG22 | 2.10 | 0.50 |
| 5:CG:465:ASN:ND2 | 5:CH:418:GLY:O | 2.42 | 0.50 |
| 5:CH:72:THR:HG22 | 5:CH:77:VAL:HG22 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:104:TYR:HE2 | 3:D:165:ARG:NH2 | 2.08 | 0.50 |
| 3:D:51:GLU:HA | 3:D:56:PHE:CD2 | 2.46 | 0.50 |
| 6:CJ:54:SER:O | 6:DA:164:GLN:NE2 | 2.43 | 0.50 |
| 7:DB:32:VAL:O | 7:DB:36:ILE:N | 2.39 | 0.50 |
| 7:DD:255:SER:HB3 | 7:DD:263:VAL:CG1 | 2.40 | 0.50 |
| 8:BB:43:ALA:HB2 | 8:DE:139:GLU:H | 1.76 | 0.50 |
| 10:DH:329:PHE:O | 10:DH:330:ASN:ND2 | 2.44 | 0.50 |
| 10:DH:323:LYS:HB3 | 10:DH:339:PRO:HG3 | 1.92 | 0.50 |
| 10:DH:332:LEU:HD21 | 10:DH:340:SER:CB | 2.41 | 0.50 |
| 12:DJ:224:SER:HB3 | 12:DJ:240:ASP:OD1 | 2.10 | 0.50 |
| 3:E:95:TRP:CD2 | 3:E:169:PRO:HB3 | 2.45 | 0.50 |
| 1:EA:287:SER:HB2 | 14:YD:373[E]:LYS:HD2 | 1.93 | 0.50 |
| 1:EA:619:GLN:HG2 | 1:EA:620:THR:HG23 | 1.92 | 0.50 |
| 1:EB:340:VAL:HG22 | 1:EB:341:THR:H | 1.77 | 0.50 |
| 2:EC:405:VAL:N | 2:EC:414:LYS:O | 2.41 | 0.50 |
| 2:EC:514:PHE:CD1 | 2:EC:525:TRP:HB2 | 2.45 | 0.50 |
| 4:EG:139:VAL:HG21 | 4:EG:146:VAL:HG21 | 1.93 | 0.50 |
| 4:EH:204:VAL:HG22 | 4:EH:276:VAL:HG22 | 1.92 | 0.50 |
| 2:EC:1000:THR:HG23 | 5:EI:17:ASP:O | 2.11 | 0.50 |
| 5:EI:407:TYR:CD2 | 5:EJ:407:TYR:CD2 | 2.99 | 0.50 |
| 5:FA:194:LYS:O | 5:FA:242:VAL:HA | 2.11 | 0.50 |
| 5:FA:359:GLU:O | 5:FA:370:HIS:N | 2.36 | 0.50 |
| 5:EI:46:ALA:N | 5:FA:65:GLY:O | 2.32 | 0.50 |
| 5:FA:72:THR:HG22 | 5:FA:77:VAL:HG22 | 1.92 | 0.50 |
| 6:FC:147:LYS:O | 6:FC:157:GLU:N | 2.44 | 0.50 |
| 7:FF:36:ILE:HG13 | 7:FG:18:PHE:CE1 | 2.46 | 0.50 |
| 9:FJ:19:TRP:CZ3 | 9:FJ:20:ASN:HB3 | 2.46 | 0.50 |
| 4:G:139:VAL:HG21 | 4:G:146:VAL:HG21 | 1.93 | 0.50 |
| 1:GE:155:ARG:NH2 | 1:GE:159:ASN:HA | 2.26 | 0.50 |
| 1:GE:340:VAL:HG22 | 1:GE:341:THR:H | 1.77 | 0.50 |
| 2:GF:233:LEU:HD23 | 2:GF:234:SER:OG | 2.10 | 0.50 |
| 2:GF:514:PHE:CD1 | 2:GF:525:TRP:HB2 | 2.45 | 0.50 |
| 2:GF:106:ASN:ND2 | 2:GF:626:GLN:HB2 | 2.26 | 0.50 |
| 5:HB:268:SER:N | 5:HB:283:THR:O | 2.35 | 0.50 |
| 5:HC:261:ARG:HB2 | 5:HC:383:ILE:HB | 1.93 | 0.50 |
| 5:HC:146:VAL:HG11 | 5:HD:151:ILE:O | 2.10 | 0.50 |
| 5:HD:180:VAL:HG13 | 5:HD:181:PHE:N | 2.26 | 0.50 |
| 5:HD:78:THR:HA | 5:HD:108:THR:HB | 1.92 | 0.50 |
| 6:HE:73:ASN:HD21 | 6:HE:215:PHE:HE2 | 1.59 | 0.50 |
| 7:HI:340:THR:HG22 | 7:HI:341:ILE:HG12 | 1.93 | 0.50 |
| 7:HH:202:GLY:HA3 | 7:HJ:216:MET:SD | 2.51 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:IF:156:ASP:O | 12:IF:245:TYR:HE2 | 1.94 | 0.50 |
| 12:IF:15:ASP:OD1 | 12:IF:16:PHE:N | 2.44 | 0.50 |
| 5:J:158:ASP:OD1 | 5:J:159:ILE:N | 2.44 | 0.50 |
| 5:J:410:GLN:HG2 | 5:J:443:PHE:O | 2.10 | 0.50 |
| 5:K:180:VAL:HG13 | 5:K:181:PHE:N | 2.26 | 0.50 |
| 5:K:275:SER:HA | 5:K:280:ILE:HG22 | 1.92 | 0.50 |
| 12:W:172:ARG:HA | 12:W:175:GLN:HB3 | 1.93 | 0.50 |
| 1:X:116:ASP:HB2 | 1:X:161:TYR:OH | 2.12 | 0.50 |
| 1:X:130:ARG:HD3 | 14:YE:181[F]:GLY:HA2 | 1.93 | 0.50 |
| 1:X:278:ALA:HA | 1:X:316:GLY:HA3 | 1.94 | 0.50 |
| 1:X:559:ALA:HB3 | 1:X:562:ASP:OD2 | 2.11 | 0.50 |
| 1:Y:348:PHE:CZ | 1:Y:399:TYR:CD2 | 2.98 | 0.50 |
| 13:YA:116[A]:ASP:OD2 | 13:YA:121[A]:TYR:N | 2.43 | 0.50 |
| 13:YA:441[D]:ILE:HG21 | 13:YB:378[D]:GLU:OE2 | 2.11 | 0.50 |
| 13:YA:13[E]:GLY:O | 13:YA:82[E]:VAL:N | 2.44 | 0.50 |
| 13:YB:379[A]:PRO:HG2 | 13:YB:429[A]:ARG:CZ | 2.41 | 0.50 |
| 13:YB:554[B]:MET:HA | 13:YC:546[B]:VAL:O | 2.11 | 0.50 |
| 13:YB:57[F]:VAL:HB | 13:YB:76[F]:PRO:HD3 | 1.93 | 0.50 |
| 13:YC:13[B]:GLY:O | 13:YC:82[B]:VAL:N | 2.44 | 0.50 |
| 13:YB:18[F]:ARG:HG3 | 13:YC:388[F]:PRO:HG3 | 1.93 | 0.50 |
| 13:YA:490[E]:VAL:O | 13:YC:498[E]:VAL:HA | 2.11 | 0.50 |
| 14:YD:101[F]:GLY:HA2 | 14:YF:332[F]:GLN:OE1 | 2.11 | 0.50 |
| 14:YD:124[F]:PHE:CE2 | 14:YD:135[F]:MET:HE2 | 2.46 | 0.50 |
| 14:YD:124[D]:PHE:CE2 | 14:YD:135[D]:MET:HE2 | 2.46 | 0.50 |
| 10:GA:285:LEU:HA | 14:YD:215[E]:GLU:CG | 2.41 | 0.50 |
| 14:YD:293[B]:GLU:N | 14:YD:293[B]:GLU:OE1 | 2.44 | 0.50 |
| 14:YD:330[D]:LYS:HE3 | 14:YD:330[D]:LYS:HA | 1.92 | 0.50 |
| 13:YB:24[E]:LEU:HD23 | 14:YE:259[E]:LEU:HD22 | 1.92 | 0.50 |
| 14:YE:330[E]:LYS:HA | 14:YE:330[E]:LYS:HE3 | 1.92 | 0.50 |
| 10:U:285:LEU:HA | 14:YF:215[C]:GLU:HG3 | 1.94 | 0.50 |
| 14:YF:293[D]:GLU:N | 14:YF:293[D]:GLU:OE1 | 2.44 | 0.50 |
| 2:Z:969:TYR:HD2 | 2:Z:982:LEU:HD13 | 1.75 | 0.50 |
| 1:A:282:GLY:N | 1:A:312:GLY:O | 2.39 | 0.50 |
| 1:A:619:GLN:HG2 | 1:A:620:THR:HG23 | 1.92 | 0.50 |
| 5:AC:64:TRP:O | 5:AC:93:ILE:HG22 | 2.10 | 0.50 |
| 5:AE:138:CYS:SG | 5:AE:140:PRO:HD2 | 2.52 | 0.50 |
| 5:AE:261:ARG:HD2 | 5:AE:297:GLY:HA3 | 1.92 | 0.50 |
| 5:AE:397:ASP:O | 5:AE:400:ILE:HG22 | 2.10 | 0.50 |
| 5:AE:460:TYR:CE2 | 5:AE:462:ASN:HB2 | 2.46 | 0.50 |
| 6:AF:19:GLY:N | 6:AG:13:ARG:NH1 | 2.59 | 0.50 |
| 6:AG:149:HIS:HB3 | 6:AG:152:ASP:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AH:73:ASN:HD21 | 6:AH:215:PHE:HE2 | 1.60 | 0.50 |
| 7:AJ:384:GLY:O | 7:AJ:391:GLY:N | 2.36 | 0.50 |
| 1:B:547:SER:O | 1:B:548:LYS:HG2 | 2.10 | 0.50 |
| 7:BA:123:VAL:O | 7:BA:127:ASN:N | 2.26 | 0.50 |
| 7:AJ:359:TRP:NE1 | 7:BA:340:THR:O | 2.36 | 0.50 |
| 7:AI:439:ILE:HG23 | 7:BA:515:TRP:CZ2 | 2.46 | 0.50 |
| 1:BH:353:PHE:HD2 | 1:BH:392:ILE:HD13 | 1.76 | 0.50 |
| 1:BH:560:SER:HA | 1:BH:588:LYS:HD3 | 1.92 | 0.50 |
| 1:BI:227:ARG:HB2 | 1:BI:237:TYR:HE2 | 1.76 | 0.50 |
| 1:BI:105:ALA:HB2 | 1:BI:275:THR:HG21 | 1.92 | 0.50 |
| 2:BJ:193:MET:HG3 | 2:BJ:238:TYR:CZ | 2.46 | 0.50 |
| 2:BJ:416:VAL:HG23 | 2:BJ:417:PHE:N | 2.25 | 0.50 |
| 2:BJ:174:HIS:CG | 2:BJ:508:TYR:HH | 2.27 | 0.50 |
| 2:BJ:969:TYR:HD2 | 2:BJ:982:LEU:HD13 | 1.75 | 0.50 |
| 2:C:581:TYR:HA | 2:C:605:ARG:HG2 | 1.93 | 0.50 |
| 2:C:701:TRP:CD2 | 2:C:701:TRP:O | 2.63 | 0.50 |
| 5:CF:100:ALA:HB2 | 5:CF:130:PHE:CD1 | 2.45 | 0.50 |
| 5:CG:204:ASP:OD1 | 5:CG:205:VAL:N | 2.41 | 0.50 |
| 5:CG:311:VAL:HG22 | 5:CG:320:LEU:HD22 | 1.92 | 0.50 |
| 5:CG:392:THR:OG1 | 5:CH:305:ASN:ND2 | 2.45 | 0.50 |
| 5:CF:1:MET:N | 5:CG:41:ASP:HB3 | 2.27 | 0.50 |
| 6:CI:35:VAL:HG13 | 6:CI:58:ASP:HB2 | 1.93 | 0.50 |
| 3:D:171:GLU:N | 3:D:171:GLU:OE1 | 2.43 | 0.50 |
| 8:DF:130:LYS:NZ | 8:DF:163:GLU:OE2 | 2.37 | 0.50 |
| 1:EB:197:VAL:HG22 | 1:EB:272:TYR:HB3 | 1.94 | 0.50 |
| 1:EB:411:PRO:HG2 | 1:EB:413:TYR:HE1 | 1.75 | 0.50 |
| 2:EC:103:PHE:CZ | 2:EC:626:GLN:O | 2.64 | 0.50 |
| 3:ED:193:GLU:O | 3:ED:223:TRP:HA | 2.11 | 0.50 |
| 5:EI:94:ARG:HD3 | 5:EI:134:GLU:HG2 | 1.93 | 0.50 |
| 5:EJ:290:SER:N | 5:EJ:371:PHE:O | 2.45 | 0.50 |
| 5:EJ:291:ILE:HG22 | 5:EJ:292:PRO:O | 2.10 | 0.50 |
| 5:EJ:419:ASP:OD1 | 5:EJ:420:VAL:N | 2.45 | 0.50 |
| 5:EJ:189:ASN:HD21 | 5:FA:150:GLN:HE22 | 1.60 | 0.50 |
| 7:FE:439:ILE:HG23 | 7:FG:515:TRP:CZ2 | 2.46 | 0.50 |
| 11:GB:45:LEU:HD23 | 11:GB:170:LYS:HB3 | 1.91 | 0.50 |
| 2:GF:405:VAL:N | 2:GF:414:LYS:O | 2.41 | 0.50 |
| 2:GF:935:LYS:HZ3 | 2:GF:936:LEU:HD13 | 1.75 | 0.50 |
| 3:GH:102:ASP:HB3 | 3:GH:105:THR:HB | 1.92 | 0.50 |
| 3:GH:122:THR:HG22 | 3:GH:169:PRO:HG2 | 1.91 | 0.50 |
| 4:GI:204:VAL:HG22 | 4:GI:276:VAL:HG22 | 1.92 | 0.50 |
| 4:GI:30:LYS:O | 4:GI:34:ASP:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:249:ASP:OD1 | 5:HC:160:SER:HB2 | 2.11 | 0.50 |
| 5:HB:446:VAL:HG21 | 5:HC:443:PHE:CD2 | 2.45 | 0.50 |
| 5:HD:257:SER:HB2 | 5:HD:387:ASN:HD22 | 1.76 | 0.50 |
| 5:I:320:LEU:HG | 5:I:357:SER:HB3 | 1.92 | 0.50 |
| 5:I:323:THR:HB | 5:I:355:ASP:HB3 | 1.93 | 0.50 |
| 5:I:322:GLY:C | 5:I:359:GLU:HA | 2.32 | 0.50 |
| 11:IE:142:LYS:HB3 | 11:IE:143:TYR:CD2 | 2.45 | 0.50 |
| 5:K:261:ARG:O | 5:K:383:ILE:N | 2.37 | 0.50 |
| 5:K:285:LEU:HD21 | 5:K:375:PHE:H | 1.76 | 0.50 |
| 6:L:147:LYS:O | 6:L:157:GLU:N | 2.44 | 0.50 |
| 6:L:35:VAL:HG13 | 6:L:58:ASP:HB2 | 1.93 | 0.50 |
| 7:O:90:ALA:HB2 | 7:O:96:GLY:CA | 2.42 | 0.50 |
| 7:O:159:ALA:HB1 | 7:P:159:ALA:HB2 | 1.94 | 0.50 |
| 7:P:84:ARG:HH12 | 7:P:88:PRO:HB3 | 1.76 | 0.50 |
| 8:R:130:LYS:NZ | 8:R:163:GLU:OE2 | 2.37 | 0.50 |
| 10:U:329:PHE:O | 10:U:330:ASN:ND2 | 2.44 | 0.50 |
| 11:V:30:ARG:HH12 | 11:V:192:TYR:HD1 | 1.56 | 0.50 |
| 1:X:400:ASN:O | 1:Y:341:THR:HA | 2.11 | 0.50 |
| 1:X:512:SER:OG | 1:X:513:ASN:N | 2.44 | 0.50 |
| 1:Y:192:ILE:HG22 | 1:Y:272:TYR:CD1 | 2.45 | 0.50 |
| 13:YA:379[D]:PRO:HG2 | 13:YA:429[D]:ARG:CZ | 2.41 | 0.50 |
| 13:YA:441[E]:ILE:HG21 | 13:YB:378[E]:GLU:OE2 | 2.11 | 0.50 |
| 13:YB:571[B]:ARG:HB3 | 13:YC:564[B]:GLN:NE2 | 2.25 | 0.50 |
| 10:ID:286:VAL:HG13 | 14:YD:100[B]:LYS:HE2 | 1.93 | 0.50 |
| 14:YD:278[F]:SER:O | 14:YD:279[F]:ARG:NH1 | 2.41 | 0.50 |
| 14:YD:293[D]:GLU:OE1 | 14:YD:293[D]:GLU:N | 2.44 | 0.50 |
| 14:YD:373[B]:LYS:HG2 | 14:YD:374[B]:ASN:N | 2.26 | 0.50 |
| 14:YE:172[D]:TYR:CE1 | 14:YE:176[D]:VAL:HG21 | 2.46 | 0.50 |
| 13:YB:24[D]:LEU:HD23 | 14:YE:259[D]:LEU:HD22 | 1.93 | 0.50 |
| 10:BE:285:LEU:HA | 14:YF:215[E]:GLU:HG3 | 1.93 | 0.50 |
| 14:YF:360[D]:ASN:H | 14:YF:360[D]:ASN:ND2 | 2.04 | 0.50 |
| 14:YE:332[E]:GLN:NE2 | 14:YF:97[E]:VAL:HG21 | 2.26 | 0.50 |
| 2:Z:416:VAL:HG23 | 2:Z:417:PHE:N | 2.25 | 0.50 |
| 2:Z:853:ASP:HB2 | 2:Z:855:ILE:HG22 | 1.92 | 0.50 |
| 15:ZA:2[C]:SER:HB3 | 15:ZA:77[C]:MET:HB3 | 1.93 | 0.50 |
| 1:A:411:PRO:HG2 | 1:A:413:TYR:HD2 | 1.77 | 0.50 |
| 5:AC:264:ARG:HG3 | 5:AC:379:ASP:O | 2.10 | 0.50 |
| 5:AC:446:VAL:HG21 | 5:AD:443:PHE:CD2 | 2.45 | 0.50 |
| 5:AE:180:VAL:HG13 | 5:AE:181:PHE:N | 2.26 | 0.50 |
| 5:AE:490:TRP:NE1 | 5:AE:500:ALA:O | 2.44 | 0.50 |
| 6:AF:4:LEU:HD23 | 6:AF:5:ASN:N | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AF:73:ASN:HD21 | 6:AF:215:PHE:HE2 | 1.59 | 0.50 |
| 7:AI:47:VAL:HG12 | 7:AI:48:PRO:N | 2.26 | 0.50 |
| 7:BA:149:GLN:O | 7:BA:153:GLY:HA2 | 2.10 | 0.50 |
| 7:AJ:36:ILE:HG13 | 7:BA:18:PHE:CE1 | 2.46 | 0.50 |
| 7:AJ:228:ILE:H | 7:BA:226:GLY:H | 1.59 | 0.50 |
| 12:BG:216:PHE:CE1 | 12:BG:218:MET:HE3 | 2.45 | 0.50 |
| 1:BH:559:ALA:HB3 | 1:BH:562:ASP:OD2 | 2.11 | 0.50 |
| 1:BH:619:GLN:HG2 | 1:BH:620:THR:HG23 | 1.92 | 0.50 |
| 1:BI:378:PRO:HG3 | 1:BI:384:LEU:HA | 1.93 | 0.50 |
| 2:BJ:1005:ARG:HG3 | 5:CF:12:ASP:OD2 | 2.12 | 0.50 |
| 2:BJ:433:ASN:HD21 | 2:BJ:513:PHE:HA | 1.75 | 0.50 |
| 2:BJ:168:ILE:HG12 | 2:BJ:578:PHE:CZ | 2.46 | 0.50 |
| 2:BJ:58:ASN:OD1 | 2:BJ:59:LEU:N | 2.44 | 0.50 |
| 2:BJ:934:ALA:HB2 | 2:BJ:998:GLY:HA2 | 1.93 | 0.50 |
| 2:BJ:947:VAL:O | 3:CA:118:PRO:HD2 | 2.11 | 0.50 |
| 2:C:17:SER:HA | 2:C:106:ASN:HB3 | 1.93 | 0.50 |
| 2:C:41:THR:O | 2:C:50:PRO:HD2 | 2.10 | 0.50 |
| 2:C:58:ASN:OD1 | 2:C:59:LEU:N | 2.44 | 0.50 |
| 3:CB:92:ARG:HD3 | 3:CB:205:ASN:O | 2.11 | 0.50 |
| 4:CC:30:LYS:O | 4:CC:34:ASP:N | 2.45 | 0.50 |
| 5:CG:158:ASP:OD1 | 5:CG:159:ILE:N | 2.44 | 0.50 |
| 7:DD:375:TYR:HE2 | 7:DD:390:PRO:HB2 | 1.77 | 0.50 |
| 7:DD:367:VAL:O | 7:DD:389:ASN:HA | 2.12 | 0.50 |
| 3:E:144:ILE:HG22 | 3:E:146:SER:H | 1.77 | 0.50 |
| 3:E:271:GLN:HB2 | 3:E:313:GLU:O | 2.11 | 0.50 |
| 1:EA:566:ASN:HB3 | 1:EA:569:ILE:HG13 | 1.94 | 0.50 |
| 2:EC:258:LYS:HG2 | 2:EC:292:GLU:HG3 | 1.92 | 0.50 |
| 2:EC:316:ASP:HA | 2:EC:331:THR:O | 2.11 | 0.50 |
| 2:EC:821:ILE:HG22 | 2:EC:822:ALA:N | 2.25 | 0.50 |
| 4:EG:204:VAL:HG22 | 4:EG:276:VAL:HG22 | 1.92 | 0.50 |
| 5:EI:262:GLN:HG2 | 5:EI:382:ASN:HD22 | 1.76 | 0.50 |
| 5:EI:334:ALA:HA | 5:EI:349:TRP:CD1 | 2.47 | 0.50 |
| 5:EI:67:SER:CB | 5:EI:94:ARG:HB2 | 2.42 | 0.50 |
| 5:EI:98:VAL:HG11 | 5:FA:89:TYR:HB3 | 1.93 | 0.50 |
| 7:FE:264:LYS:O | 7:FE:279:SER:HA | 2.11 | 0.50 |
| 7:FF:228:ILE:O | 7:FG:225:LYS:HA | 2.11 | 0.50 |
| 7:FF:78:PRO:HB2 | 7:FG:69:GLY:HA2 | 1.93 | 0.50 |
| 7:FG:149:GLN:O | 7:FG:153:GLY:HA2 | 2.10 | 0.50 |
| 7:FG:289:GLN:OE1 | 7:FG:294:GLN:NE2 | 2.41 | 0.50 |
| 7:FG:20:PRO:HD3 | 7:FG:29:ILE:HG21 | 1.92 | 0.50 |
| 7:FE:504:ARG:HA | 7:FG:422:LYS:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:GA:222:ILE:O | 10:GA:225:ILE:HG22 | 2.12 | 0.50 |
| 2:EC:713:ILE:HD12 | 1:GE:427:ASN:HA | 1.93 | 0.50 |
| 1:GE:52:ARG:HE | 9:IC:13:PRO:HB3 | 1.76 | 0.50 |
| 2:GF:316:ASP:HA | 2:GF:331:THR:O | 2.11 | 0.50 |
| 2:GF:853:ASP:HB2 | 2:GF:855:ILE:HG22 | 1.92 | 0.50 |
| 2:GF:947:VAL:O | 3:GG:118:PRO:HD2 | 2.12 | 0.50 |
| 3:GG:225:TYR:CE2 | 3:GG:231:TRP:HB3 | 2.47 | 0.50 |
| 3:GH:144:ILE:HG22 | 3:GH:146:SER:H | 1.77 | 0.50 |
| 3:GH:271:GLN:HB2 | 3:GH:313:GLU:O | 2.11 | 0.50 |
| 3:GH:95:TRP:CD2 | 3:GH:169:PRO:HB3 | 2.45 | 0.50 |
| 5:HC:551:ILE:HD13 | 5:HD:565:ILE:CD1 | 2.41 | 0.50 |
| 5:HD:193:VAL:O | 5:HD:199:GLU:N | 2.37 | 0.50 |
| 6:HE:149:HIS:HB3 | 6:HE:152:ASP:O | 2.11 | 0.50 |
| 6:HE:4:LEU:HD23 | 6:HE:5:ASN:N | 2.27 | 0.50 |
| 6:HF:147:LYS:O | 6:HF:157:GLU:N | 2.44 | 0.50 |
| 7:HH:349:TRP:CZ3 | 7:HI:342:PRO:HG2 | 2.46 | 0.50 |
| 7:HH:76:VAL:HG11 | 7:HJ:81:LEU:HD22 | 1.93 | 0.50 |
| 7:HH:90:ALA:HB2 | 7:HH:96:GLY:CA | 2.42 | 0.50 |
| 7:HH:476:ASP:OD2 | 7:HI:454:HIS:HE1 | 1.95 | 0.50 |
| 1:GD:69:GLN:HE21 | 11:IE:25:MET:CE | 2.23 | 0.50 |
| 5:K:194:LYS:O | 5:K:242:VAL:HA | 2.11 | 0.50 |
| 6:L:73:ASN:HD21 | 6:L:215:PHE:HE2 | 1.59 | 0.50 |
| 6:L:13:ARG:NH1 | 6:N:47:PHE:CE1 | 2.79 | 0.50 |
| 9:T:19:TRP:CZ3 | 9:T:20:ASN:HB3 | 2.46 | 0.50 |
| 12:W:216:PHE:HE1 | 12:W:218:MET:CE | 2.23 | 0.50 |
| 1:X:539:ARG:CD | 1:X:580:LEU:HD23 | 2.41 | 0.50 |
| 1:Y:80:MET:HG3 | 1:Y:81:ARG:HG3 | 1.94 | 0.50 |
| 13:YA:529[D]:THR:N | 13:YB:520[D]:THR:O | 2.44 | 0.50 |
| 13:YA:95[F]:ILE:HD11 | 13:YB:83[F]:TYR:CZ | 2.46 | 0.50 |
| 13:YB:436[A]:ASP:OD2 | 13:YB:437[A]:ASN:N | 2.44 | 0.50 |
| 13:YA:529[E]:THR:N | 13:YB:520[E]:THR:O | 2.44 | 0.50 |
| 13:YA:538[C]:VAL:HG21 | 13:YB:534[C]:LEU:HD22 | 1.94 | 0.50 |
| 13:YB:554[F]:MET:HA | 13:YC:546[F]:VAL:O | 2.11 | 0.50 |
| 13:YB:61[C]:ILE:HA | 13:YC:76[C]:PRO:C | 2.31 | 0.50 |
| 13:YB:13[F]:GLY:O | 13:YB:82[F]:VAL:N | 2.45 | 0.50 |
| 13:YC:13[F]:GLY:O | 13:YC:82[F]:VAL:N | 2.45 | 0.50 |
| 13:YC:179[D]:MET:SD | 13:YC:279[D]:ASN:ND2 | 2.76 | 0.50 |
| 13:YC:179[E]:MET:SD | 13:YC:279[E]:ASN:ND2 | 2.76 | 0.50 |
| 13:YC:270[F]:ASN:O | 13:YC:274[F]:GLN:N | 2.42 | 0.50 |
| 13:YC:344[B]:LYS:HE2 | 13:YC:344[B]:LYS:HA | 1.93 | 0.50 |
| 14:YE:293[A]:GLU:N | 14:YE:293[A]:GLU:OE1 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:373[E]:LYS:HG2 | 14:YE:374[E]:ASN:N | 2.26 | 0.50 |
| 14:YF:293[C]:GLU:N | 14:YF:293[C]:GLU:OE1 | 2.44 | 0.50 |
| 14:YF:373[C]:LYS:HG2 | 14:YF:374[C]:ASN:N | 2.26 | 0.50 |
| 2:Z:379:ILE:HG13 | 2:Z:402:GLY:O | 2.10 | 0.50 |
| 2:Z:581:TYR:HA | 2:Z:605:ARG:HG2 | 1.93 | 0.50 |
| 1:A:278:ALA:HA | 1:A:316:GLY:HA3 | 1.94 | 0.50 |
| 5:AC:320:LEU:HG | 5:AC:357:SER:HB3 | 1.92 | 0.50 |
| 5:AC:289:LYS:HE2 | 5:AC:370:HIS:CE1 | 2.47 | 0.50 |
| 5:AC:568:LYS:HA | 5:AD:550:VAL:O | 2.11 | 0.50 |
| 5:AC:86:VAL:HG13 | 5:AC:87:ASN:N | 2.26 | 0.50 |
| 5:AD:261:ARG:HB2 | 5:AD:383:ILE:HB | 1.93 | 0.50 |
| 6:AH:147:LYS:O | 6:AH:157:GLU:N | 2.44 | 0.50 |
| 6:AH:4:LEU:HD23 | 6:AH:5:ASN:N | 2.27 | 0.50 |
| 7:AJ:220:SER:OG | 7:AJ:226:GLY:O | 2.28 | 0.50 |
| 1:B:411:PRO:HG2 | 1:B:413:TYR:HE1 | 1.75 | 0.50 |
| 7:AJ:295:ILE:HG12 | 7:BA:301:ARG:HD3 | 1.93 | 0.50 |
| 8:BB:14:ASP:OD2 | 8:BB:17:ARG:NH2 | 2.33 | 0.50 |
| 8:BC:137:VAL:HA | 8:BC:155:VAL:HG12 | 1.94 | 0.50 |
| 1:BH:67:ILE:CD1 | 1:BI:67:ILE:HG21 | 2.42 | 0.50 |
| 1:BI:197:VAL:HG22 | 1:BI:272:TYR:HB3 | 1.94 | 0.50 |
| 1:BI:98:TYR:CE2 | 1:BI:100:PRO:HA | 2.47 | 0.50 |
| 2:BJ:935:LYS:HZ2 | 2:BJ:936:LEU:HD13 | 1.75 | 0.50 |
| 2:C:1014:ASP:CG | 2:C:1015:ASN:H | 2.15 | 0.50 |
| 2:C:514:PHE:CD1 | 2:C:525:TRP:HB2 | 2.45 | 0.50 |
| 3:CA:104:TYR:HE2 | 3:CA:165:ARG:NH2 | 2.08 | 0.50 |
| 3:CA:7:ILE:HD11 | 3:CB:316:PRO:HG2 | 1.93 | 0.50 |
| 3:CB:102:ASP:HB3 | 3:CB:105:THR:HB | 1.92 | 0.50 |
| 4:CD:53:GLY:HA3 | 4:CE:7:LYS:HE2 | 1.94 | 0.50 |
| 5:CG:261:ARG:HB2 | 5:CG:383:ILE:HB | 1.93 | 0.50 |
| 5:CH:460:TYR:CE2 | 5:CH:462:ASN:HB2 | 2.46 | 0.50 |
| 6:CI:149:HIS:HB3 | 6:CI:152:ASP:O | 2.11 | 0.50 |
| 6:CI:4:LEU:HD23 | 6:CI:5:ASN:N | 2.27 | 0.50 |
| 6:CJ:73:ASN:HD21 | 6:CJ:215:PHE:HE2 | 1.59 | 0.50 |
| 2:C:1013:LYS:HB3 | 3:D:206:GLU:OE2 | 2.12 | 0.50 |
| 3:D:225:TYR:CE2 | 3:D:231:TRP:HB3 | 2.47 | 0.50 |
| 7:DC:220:SER:OG | 7:DC:226:GLY:O | 2.28 | 0.50 |
| 7:DB:265:LEU:O | 7:DC:257:THR:HA | 2.11 | 0.50 |
| 7:DC:476:ASP:OD1 | 7:DC:479:ASN:ND2 | 2.40 | 0.50 |
| 10:DH:222:ILE:O | 10:DH:225:ILE:HG22 | 2.12 | 0.50 |
| 12:DJ:159:VAL:HG22 | 12:DJ:242:THR:HG22 | 1.93 | 0.50 |
| 1:EB:123:ILE:HG12 | 1:EB:161:TYR:OH | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:336:GLN:HG2 | 1:EB:336:GLN:HG2 | 1.94 | 0.50 |
| 1:EB:461:LYS:HE3 | 1:EB:630:ASP:OD1 | 2.12 | 0.50 |
| 3:EE:102:ASP:HB3 | 3:EE:105:THR:HB | 1.92 | 0.50 |
| 3:EE:144:ILE:HG22 | 3:EE:146:SER:H | 1.77 | 0.50 |
| 4:EF:284:ILE:HD11 | 4:EH:205:THR:HG22 | 1.93 | 0.50 |
| 5:EI:289:LYS:HE2 | 5:EI:370:HIS:CE1 | 2.47 | 0.50 |
| 5:EJ:158:ASP:OD1 | 5:EJ:159:ILE:N | 2.44 | 0.50 |
| 5:EJ:180:VAL:HG13 | 5:EJ:181:PHE:N | 2.25 | 0.50 |
| 5:FA:223:VAL:HB | 5:FA:224:PRO:HD3 | 1.92 | 0.50 |
| 5:FA:192:ARG:HG3 | 5:FA:245:GLU:HB2 | 1.93 | 0.50 |
| 6:FC:122:ALA:O | 6:FC:126:VAL:HG23 | 2.12 | 0.50 |
| 5:EI:340:VAL:HG21 | 6:FC:174:TYR:H | 1.76 | 0.50 |
| 7:FE:106:ALA:HB2 | 7:FE:120:LYS:HD2 | 1.94 | 0.50 |
| 8:FH:6:VAL:HB | 8:FI:53:PHE:CD1 | 2.46 | 0.50 |
| 2:C:58:ASN:HB3 | 4:G:155:ASN:HD21 | 1.77 | 0.50 |
| 1:GD:336:GLN:HG2 | 1:GE:336:GLN:HG2 | 1.94 | 0.50 |
| 1:GD:344:ASP:O | 1:GD:347:THR:N | 2.44 | 0.50 |
| 1:GE:424:TYR:OH | 1:GE:657:PRO:HG3 | 2.11 | 0.50 |
| 2:GF:182:GLN:O | 2:GF:210:LYS:NZ | 2.33 | 0.50 |
| 4:GI:205:THR:HG22 | 4:GJ:284:ILE:HD11 | 1.93 | 0.50 |
| 4:GJ:131:LYS:HD3 | 4:GJ:161:ASN:ND2 | 2.25 | 0.50 |
| 4:GJ:205:THR:HG22 | 4:HA:284:ILE:HD11 | 1.92 | 0.50 |
| 4:H:139:VAL:HG21 | 4:H:146:VAL:HG21 | 1.94 | 0.50 |
| 5:HB:322:GLY:C | 5:HB:359:GLU:HA | 2.32 | 0.50 |
| 7:HH:485:ASN:C | 7:HI:446:LYS:HG2 | 2.32 | 0.50 |
| 7:HI:14:ARG:HG2 | 7:HI:33:GLN:HG2 | 1.93 | 0.50 |
| 7:HI:371:ASP:OD1 | 7:HI:526:LYS:NZ | 2.45 | 0.50 |
| 7:HI:367:VAL:O | 7:HI:389:ASN:HA | 2.10 | 0.50 |
| 5:I:194:LYS:HE3 | 5:K:198:ASN:HD22 | 1.75 | 0.50 |
| 5:I:196:ARG:HD3 | 7:O:5:THR:HG23 | 1.91 | 0.50 |
| 5:I:94:ARG:HD3 | 5:I:134:GLU:HG2 | 1.93 | 0.50 |
| 9:IC:19:TRP:CZ3 | 9:IC:20:ASN:HB3 | 2.46 | 0.50 |
| 10:ID:208:THR:HA | 10:ID:345:GLU:HG2 | 1.94 | 0.50 |
| 5:I:7:ILE:HG12 | 5:J:24:ILE:HG13 | 1.94 | 0.50 |
| 5:J:264:ARG:HG3 | 5:J:379:ASP:O | 2.12 | 0.50 |
| 5:K:223:VAL:HB | 5:K:224:PRO:HD3 | 1.93 | 0.50 |
| 6:N:4:LEU:HD23 | 6:N:5:ASN:N | 2.27 | 0.50 |
| 6:N:73:ASN:HD21 | 6:N:215:PHE:HE2 | 1.60 | 0.50 |
| 7:O:233:GLN:CG | 5:HB:348:THR:H | 2.24 | 0.50 |
| 7:O:47:VAL:HG12 | 7:O:48:PRO:N | 2.26 | 0.50 |
| 7:P:228:ILE:H | 7:Q:226:GLY:H | 1.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:340:THR:HG22 | 7:P:341:ILE:HG12 | 1.93 | 0.50 |
| 7:P:367:VAL:O | 7:P:389:ASN:HA | 2.10 | 0.50 |
| 7:Q:375:TYR:CE2 | 7:Q:390:PRO:HB2 | 2.45 | 0.50 |
| 9:T:105:ILE:HA | 9:T:125:GLN:HA | 1.93 | 0.50 |
| 1:X:560:SER:HA | 1:X:588:LYS:HD3 | 1.92 | 0.50 |
| 1:X:627:PRO:HG3 | 1:X:632:ILE:HD11 | 1.92 | 0.50 |
| 1:Y:227:ARG:HB2 | 1:Y:237:TYR:HE2 | 1.76 | 0.50 |
| 1:Y:424:TYR:OH | 1:Y:657:PRO:HG3 | 2.11 | 0.50 |
| 13:YA:367[B]:PRO:HA | 13:YC:315[B]:LEU:HD23 | 1.92 | 0.50 |
| 13:YA:379[E]:PRO:HG2 | 13:YA:429[E]:ARG:CZ | 2.40 | 0.50 |
| 13:YA:430[A]:ARG:HB3 | 13:YC:434[A]:THR:HG21 | 1.93 | 0.50 |
| 13:YA:490[F]:VAL:O | 13:YC:498[F]:VAL:HA | 2.11 | 0.50 |
| 13:YA:82[F]:VAL:HG22 | 13:YA:98[F]:GLY:O | 2.10 | 0.50 |
| 13:YC:109[D]:ASN:HB3 | 13:YC:112[D]:GLU:HB2 | 1.94 | 0.50 |
| 13:YB:554[C]:MET:HA | 13:YC:546[C]:VAL:O | 2.11 | 0.50 |
| 10:U:285:LEU:HA | 14:YD:215[A]:GLU:HG3 | 1.94 | 0.50 |
| 14:YD:360[B]:ASN:ND2 | 14:YD:360[B]:ASN:H | 2.04 | 0.50 |
| 1:A:130:ARG:HD3 | 14:YE:181[E]:GLY:HA2 | 1.92 | 0.50 |
| 14:YE:293[B]:GLU:OE1 | 14:YE:293[B]:GLU:N | 2.45 | 0.50 |
| 1:BH:287:SER:HB2 | 14:YE:373[B]:LYS:HD2 | 1.93 | 0.50 |
| 14:YE:373[F]:LYS:HG2 | 14:YE:374[F]:ASN:N | 2.27 | 0.50 |
| 14:YF:360[A]:ASN:H | 14:YF:360[A]:ASN:ND2 | 2.04 | 0.50 |
| 1:A:353:PHE:HD2 | 1:A:392:ILE:HD13 | 1.76 | 0.50 |
| 1:A:543:THR:OG1 | 1:A:544:ASP:N | 2.45 | 0.50 |
| 4:AA:30:LYS:O | 4:AA:34:ASP:N | 2.45 | 0.50 |
| 5:AC:175:THR:O | 5:AC:232:LEU:N | 2.35 | 0.50 |
| 5:AC:20:ARG:CZ | 5:AE:7:ILE:HD12 | 2.41 | 0.50 |
| 5:AD:159:ILE:HG23 | 5:AD:246:THR:HG21 | 1.94 | 0.50 |
| 5:AD:158:ASP:OD1 | 5:AD:159:ILE:N | 2.44 | 0.50 |
| 5:AD:202:TYR:OH | 5:AD:223:VAL:O | 2.19 | 0.50 |
| 5:AD:290:SER:N | 5:AD:371:PHE:O | 2.45 | 0.50 |
| 6:AF:140:PHE:CZ | 7:DC:196:VAL:HG11 | 2.46 | 0.50 |
| 7:AI:359:TRP:NE1 | 7:AJ:340:THR:O | 2.29 | 0.50 |
| 10:BE:329:PHE:O | 10:BE:330:ASN:ND2 | 2.44 | 0.50 |
| 11:BF:2:LEU:O | 11:BF:4:THR:N | 2.45 | 0.50 |
| 1:BH:512:SER:OG | 1:BH:513:ASN:N | 2.44 | 0.50 |
| 1:BI:106:ALA:HB2 | 1:BI:280:ALA:HB1 | 1.93 | 0.50 |
| 2:BJ:1014:ASP:CG | 2:BJ:1015:ASN:H | 2.15 | 0.50 |
| 2:BJ:357:ILE:HG12 | 2:BJ:358:THR:H | 1.77 | 0.50 |
| 2:BJ:231:TYR:HE2 | 2:BJ:389:ASN:HD21 | 1.58 | 0.50 |
| 2:C:103:PHE:CZ | 2:C:626:GLN:O | 2.64 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CC:139:VAL:HG21 | 4:CC:146:VAL:HG21 | 1.94 | 0.50 |
| 5:CF:194:LYS:HB2 | 5:CF:243:GLN:HB2 | 1.92 | 0.50 |
| 5:CF:289:LYS:HE2 | 5:CF:370:HIS:CE1 | 2.47 | 0.50 |
| 5:CH:180:VAL:HG13 | 5:CH:181:PHE:N | 2.26 | 0.50 |
| 5:CH:285:LEU:HD21 | 5:CH:375:PHE:H | 1.76 | 0.50 |
| 6:CJ:149:HIS:HB3 | 6:CJ:152:ASP:O | 2.11 | 0.50 |
| 3:D:193:GLU:O | 3:D:223:TRP:HA | 2.11 | 0.50 |
| 7:DB:145:SER:O | 7:DB:164:LYS:HE2 | 2.11 | 0.50 |
| 7:DB:451:PHE:HD1 | 7:DB:469:VAL:HG13 | 1.75 | 0.50 |
| 7:DB:452:GLY:HA2 | 7:DD:482:TYR:CD2 | 2.47 | 0.50 |
| 7:DB:480:ARG:NE | 7:DC:465:ARG:HG3 | 2.26 | 0.50 |
| 7:DB:493:GLU:HA | 7:DB:496:ARG:HH21 | 1.76 | 0.50 |
| 10:DH:132:SER:HA | 10:DH:209:TRP:NE1 | 2.25 | 0.50 |
| 12:DJ:220:SER:HA | 12:DJ:243:PHE:CD1 | 2.47 | 0.50 |
| 3:E:89:VAL:HG12 | 3:E:209:VAL:HA | 1.94 | 0.50 |
| 2:EC:191:TYR:CE1 | 2:EC:235:LYS:HA | 2.47 | 0.50 |
| 3:ED:51:GLU:HA | 3:ED:56:PHE:CD2 | 2.46 | 0.50 |
| 4:EF:61:ILE:O | 4:EG:4:GLN:NE2 | 2.42 | 0.50 |
| 4:EG:131:LYS:HD3 | 4:EG:161:ASN:ND2 | 2.25 | 0.50 |
| 5:EI:190:ASN:CB | 5:EI:247:PHE:HB2 | 2.41 | 0.50 |
| 5:EJ:264:ARG:HG3 | 5:EJ:379:ASP:O | 2.12 | 0.50 |
| 5:EJ:311:VAL:HG22 | 5:EJ:320:LEU:HD22 | 1.92 | 0.50 |
| 5:EJ:261:ARG:HB2 | 5:EJ:383:ILE:HB | 1.93 | 0.50 |
| 7:FE:493:GLU:HA | 7:FE:496:ARG:HH21 | 1.76 | 0.50 |
| 5:EI:196:ARG:HH11 | 7:FE:5:THR:HG23 | 1.77 | 0.50 |
| 4:F:39:TYR:CG | 4:G:7:LYS:HD3 | 2.46 | 0.50 |
| 10:GA:329:PHE:O | 10:GA:330:ASN:ND2 | 2.44 | 0.50 |
| 10:GA:340:SER:O | 10:GA:341:THR:HG23 | 2.11 | 0.50 |
| 1:GD:460:ALA:HA | 1:GD:631:VAL:HG12 | 1.93 | 0.50 |
| 1:GD:525:ASN:O | 1:GD:528:THR:OG1 | 2.11 | 0.50 |
| 1:GD:566:ASN:HB3 | 1:GD:569:ILE:HG13 | 1.94 | 0.50 |
| 1:GE:227:ARG:HB2 | 1:GE:237:TYR:HE2 | 1.76 | 0.50 |
| 1:GE:197:VAL:HG22 | 1:GE:272:TYR:HB3 | 1.94 | 0.50 |
| 1:GE:76:TYR:CE2 | 11:IE:31:ASN:HA | 2.47 | 0.50 |
| 2:GF:103:PHE:CZ | 2:GF:626:GLN:O | 2.64 | 0.50 |
| 2:GF:6:PRO:O | 2:GF:7:SER:OG | 2.27 | 0.50 |
| 5:HB:67:SER:CB | 5:HB:94:ARG:HB2 | 2.42 | 0.50 |
| 2:GF:984:SER:OG | 5:HC:12:ASP:OD2 | 2.14 | 0.50 |
| 5:HC:415:ASP:HB2 | 5:HC:440:GLN:HE22 | 1.76 | 0.50 |
| 6:HE:35:VAL:HG13 | 6:HE:58:ASP:HB2 | 1.93 | 0.50 |
| 6:HF:82:VAL:HB | 6:HF:187:LYS:HB3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:424:ARG:O | 7:HJ:504:ARG:NH2 | 2.35 | 0.50 |
| 7:HI:36:ILE:HG13 | 7:HJ:18:PHE:CE1 | 2.47 | 0.50 |
| 5:I:289:LYS:HE2 | 5:I:370:HIS:CE1 | 2.47 | 0.50 |
| 5:I:76:ARG:NH2 | 5:I:78:THR:OG1 | 2.45 | 0.50 |
| 10:ID:222:ILE:O | 10:ID:225:ILE:HG22 | 2.12 | 0.50 |
| 12:IF:220:SER:HA | 12:IF:243:PHE:CD1 | 2.47 | 0.50 |
| 2:C:977:ILE:HD13 | 5:J:12:ASP:HB3 | 1.94 | 0.50 |
| 6:M:122:ALA:O | 6:M:126:VAL:HG23 | 2.12 | 0.50 |
| 6:N:82:VAL:HB | 6:N:187:LYS:HB3 | 1.92 | 0.50 |
| 7:O:145:SER:O | 7:O:164:LYS:HE2 | 2.11 | 0.50 |
| 7:P:167:GLN:O | 7:P:170:ILE:N | 2.45 | 0.50 |
| 7:Q:211:SER:N | 7:Q:214:THR:OG1 | 2.39 | 0.50 |
| 11:V:147:GLU:OE1 | 11:V:147:GLU:N | 2.45 | 0.50 |
| 11:V:2:LEU:O | 11:V:4:THR:N | 2.45 | 0.50 |
| 12:W:156:ASP:O | 12:W:245:TYR:HE2 | 1.94 | 0.50 |
| 12:W:220:SER:HA | 12:W:243:PHE:CD1 | 2.47 | 0.50 |
| 1:Y:187:ILE:HD11 | 1:Y:270:ILE:HD13 | 1.93 | 0.50 |
| 13:YA:430[C]:ARG:HB3 | 13:YC:434[C]:THR:HG21 | 1.93 | 0.50 |
| 13:YA:473[A]:GLN:HA | 13:YC:481[A]:PHE:O | 2.12 | 0.50 |
| 13:YA:490[B]:VAL:O | 13:YC:498[B]:VAL:HA | 2.11 | 0.50 |
| 13:YA:529[C]:THR:N | 13:YB:520[C]:THR:O | 2.44 | 0.50 |
| 13:YB:109[A]:ASN:HB3 | 13:YB:112[A]:GLU:HB2 | 1.94 | 0.50 |
| 13:YB:109[E]:ASN:HB3 | 13:YB:112[E]:GLU:HB2 | 1.93 | 0.50 |
| 13:YB:24[B]:LEU:HD23 | 14:YE:259[B]:LEU:HD22 | 1.92 | 0.50 |
| 13:YB:571[C]:ARG:HD3 | 13:YC:564[C]:GLN:HE22 | 1.77 | 0.50 |
| 13:YC:344[A]:LYS:HA | 13:YC:344[A]:LYS:HE2 | 1.93 | 0.50 |
| 13:YC:416[E]:HIS:CE1 | 13:YC:417[E]:PRO:HD2 | 2.47 | 0.50 |
| 13:YA:428[C]:GLY:HA3 | 13:YC:418[C]:THR:HG21 | 1.93 | 0.50 |
| 13:YA:473[B]:GLN:HA | 13:YC:481[B]:PHE:O | 2.12 | 0.50 |
| 14:YD:296[C]:ILE:HD11 | 14:YD:367[C]:ILE:HA | 1.93 | 0.50 |
| 14:YE:293[C]:GLU:N | 14:YE:293[C]:GLU:OE1 | 2.44 | 0.50 |
| 14:YF:293[E]:GLU:OE1 | 14:YF:293[E]:GLU:N | 2.45 | 0.50 |
| 2:Z:916:TYR:HB3 | 2:Z:1004:PHE:HB3 | 1.94 | 0.50 |
| 2:Z:17:SER:HA | 2:Z:106:ASN:HB3 | 1.93 | 0.50 |
| 2:Z:168:ILE:HG12 | 2:Z:578:PHE:CZ | 2.46 | 0.50 |
| 1:A:116:ASP:HB2 | 1:A:161:TYR:OH | 2.12 | 0.50 |
| 1:A:336:GLN:HG2 | 1:B:336:GLN:HG2 | 1.94 | 0.50 |
| 5:AC:334:ALA:HA | 5:AC:349:TRP:CD1 | 2.47 | 0.50 |
| 5:AC:76:ARG:NH2 | 5:AC:78:THR:OG1 | 2.45 | 0.50 |
| 5:AD:168:LEU:HA | 5:AD:241:THR:HG22 | 1.94 | 0.50 |
| 5:AE:395:THR:HG22 | 5:AE:396:LYS:H | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AF:200:THR:OG1 | 6:AG:204:ASP:OD2 | 2.27 | 0.50 |
| 6:AG:73:ASN:HD21 | 6:AG:215:PHE:HE2 | 1.60 | 0.50 |
| 7:AI:482:TYR:OH | 7:AJ:453:GLU:HB2 | 2.12 | 0.50 |
| 7:AJ:451:PHE:CE1 | 7:AJ:470:GLY:HA2 | 2.46 | 0.50 |
| 7:AJ:84:ARG:HH12 | 7:AJ:88:PRO:HB3 | 1.76 | 0.50 |
| 1:B:227:ARG:HB2 | 1:B:237:TYR:HE2 | 1.76 | 0.50 |
| 1:B:340:VAL:HG22 | 1:B:341:THR:H | 1.77 | 0.50 |
| 1:B:80:MET:HG3 | 1:B:81:ARG:HG3 | 1.94 | 0.50 |
| 10:BE:332:LEU:HD21 | 10:BE:340:SER:CB | 2.41 | 0.50 |
| 11:BF:147:GLU:OE1 | 11:BF:147:GLU:N | 2.45 | 0.50 |
| 12:BG:224:SER:HB3 | 12:BG:240:ASP:OD1 | 2.11 | 0.50 |
| 1:BH:411:PRO:HG2 | 1:BH:413:TYR:HD2 | 1.77 | 0.50 |
| 1:BI:114:CYS:HG | 1:BI:161:TYR:HH | 1.59 | 0.50 |
| 1:BI:80:MET:HG3 | 1:BI:81:ARG:HG3 | 1.94 | 0.50 |
| 2:BJ:106:ASN:ND2 | 2:BJ:626:GLN:HB2 | 2.26 | 0.50 |
| 2:BJ:238:TYR:HB3 | 2:BJ:247:VAL:HG12 | 1.94 | 0.50 |
| 2:BJ:816:LEU:HB2 | 3:CB:201:ASN:HD22 | 1.75 | 0.50 |
| 2:C:371:ILE:HG13 | 2:C:372:CYS:H | 1.76 | 0.50 |
| 3:CA:50:ASN:HB2 | 3:CA:56:PHE:CE1 | 2.47 | 0.50 |
| 3:CB:61:PRO:HG3 | 3:CB:314:ASN:OD1 | 2.12 | 0.50 |
| 4:CD:139:VAL:HG21 | 4:CD:146:VAL:HG21 | 1.93 | 0.50 |
| 5:CF:94:ARG:HD3 | 5:CF:134:GLU:HG2 | 1.93 | 0.50 |
| 5:CF:161:ASN:HB2 | 5:CF:248:MET:SD | 2.52 | 0.50 |
| 5:CF:563:GLY:HA3 | 5:CF:566:TYR:OH | 2.12 | 0.50 |
| 5:CF:486:VAL:HG22 | 5:CH:591:PRO:O | 2.12 | 0.50 |
| 6:CI:122:ALA:O | 6:CI:126:VAL:HG23 | 2.12 | 0.50 |
| 3:D:108:ILE:HD12 | 3:D:108:ILE:H | 1.75 | 0.50 |
| 7:DB:90:ALA:HB2 | 7:DB:96:GLY:CA | 2.42 | 0.50 |
| 11:DI:138:ASP:HB3 | 11:DI:140:ALA:H | 1.77 | 0.50 |
| 3:D:63:ASP:HB2 | 3:E:13:THR:HG23 | 1.93 | 0.50 |
| 1:EA:559:ALA:HB3 | 1:EA:562:ASP:OD2 | 2.11 | 0.50 |
| 1:EB:444:ILE:O | 1:EB:447:TYR:N | 2.45 | 0.50 |
| 2:EC:168:ILE:HG12 | 2:EC:578:PHE:CZ | 2.46 | 0.50 |
| 2:EC:977:ILE:HD13 | 5:EJ:12:ASP:HB3 | 1.93 | 0.50 |
| 3:EE:271:GLN:HB2 | 3:EE:313:GLU:O | 2.11 | 0.50 |
| 4:EH:30:LYS:O | 4:EH:34:ASP:N | 2.45 | 0.50 |
| 5:EI:289:LYS:O | 5:EI:290:SER:OG | 2.24 | 0.50 |
| 6:FB:82:VAL:HB | 6:FB:187:LYS:HB3 | 1.92 | 0.50 |
| 6:FB:35:VAL:HG13 | 6:FB:58:ASP:HB2 | 1.93 | 0.50 |
| 6:FD:149:HIS:HB3 | 6:FD:152:ASP:O | 2.11 | 0.50 |
| 7:FE:27:PRO:HA | 7:FE:29:ILE:HD11 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:111:ASN:HD21 | 4:G:115:SER:N | 2.10 | 0.50 |
| 4:G:204:VAL:HG22 | 4:G:276:VAL:HG22 | 1.92 | 0.50 |
| 11:GB:61:ASN:O | 11:GB:65:GLY:N | 2.38 | 0.50 |
| 1:GD:400:ASN:O | 1:GE:341:THR:HA | 2.12 | 0.50 |
| 1:GE:80:MET:HG3 | 1:GE:81:ARG:HG3 | 1.94 | 0.50 |
| 1:GE:86:ARG:HG3 | 1:GE:322:ILE:HG22 | 1.93 | 0.50 |
| 3:GG:108:ILE:HD12 | 3:GG:108:ILE:H | 1.76 | 0.50 |
| 3:GG:51:GLU:HA | 3:GG:56:PHE:CD2 | 2.46 | 0.50 |
| 4:H:204:VAL:HG22 | 4:H:276:VAL:HG22 | 1.92 | 0.50 |
| 5:HB:289:LYS:HE2 | 5:HB:370:HIS:CE1 | 2.47 | 0.50 |
| 5:HC:200:LEU:HD11 | 5:HD:241:THR:HG21 | 1.94 | 0.50 |
| 5:HD:490:TRP:CD1 | 5:HD:516:ALA:HA | 2.46 | 0.50 |
| 6:HF:4:LEU:HD23 | 6:HF:5:ASN:N | 2.27 | 0.50 |
| 6:HG:149:HIS:HB3 | 6:HG:152:ASP:O | 2.11 | 0.50 |
| 7:HH:511:GLU:HB3 | 7:HH:513:ARG:HH11 | 1.74 | 0.50 |
| 5:I:161:ASN:HB2 | 5:I:248:MET:SD | 2.52 | 0.50 |
| 5:I:267:ASP:OD1 | 5:I:285:LEU:HB2 | 2.11 | 0.50 |
| 12:IF:224:SER:HB3 | 12:IF:240:ASP:OD1 | 2.11 | 0.50 |
| 5:J:392:THR:OG1 | 5:K:305:ASN:ND2 | 2.45 | 0.50 |
| 5:J:415:ASP:HB2 | 5:J:440:GLN:HE22 | 1.77 | 0.50 |
| 5:K:192:ARG:HG3 | 5:K:245:GLU:HB2 | 1.93 | 0.50 |
| 5:K:395:THR:HG22 | 5:K:396:LYS:H | 1.77 | 0.50 |
| 5:K:501:LEU:HB3 | 5:K:512:PRO:HB2 | 1.94 | 0.50 |
| 7:O:160:MET:SD | 7:O:165:THR:HB | 2.52 | 0.50 |
| 12:W:15:ASP:OD1 | 12:W:16:PHE:N | 2.44 | 0.50 |
| 1:Y:510:MET:SD | 1:Y:602:ILE:HD13 | 2.52 | 0.50 |
| 13:YA:344[F]:LYS:HA | 13:YA:344[F]:LYS:HE2 | 1.94 | 0.50 |
| 13:YA:416[C]:HIS:CE1 | 13:YA:417[C]:PRO:HD2 | 2.47 | 0.50 |
| 13:YA:436[A]:ASP:OD2 | 13:YA:437[A]:ASN:N | 2.44 | 0.50 |
| 13:YA:538[E]:VAL:HG21 | 13:YB:534[E]:LEU:HD22 | 1.94 | 0.50 |
| 13:YA:66[A]:MET:O | 13:YA:69[A]:ILE:N | 2.44 | 0.50 |
| 13:YB:344[C]:LYS:HA | 13:YB:344[C]:LYS:HE2 | 1.94 | 0.50 |
| 13:YB:416[B]:HIS:CE1 | 13:YB:417[B]:PRO:HD2 | 2.47 | 0.50 |
| 13:YB:554[E]:MET:HA | 13:YC:546[E]:VAL:O | 2.11 | 0.50 |
| 13:YC:179[C]:MET:SD | 13:YC:279[C]:ASN:ND2 | 2.76 | 0.50 |
| 13:YC:416[F]:HIS:CE1 | 13:YC:417[F]:PRO:HD2 | 2.47 | 0.50 |
| 13:YB:442[C]:THR:HG21 | 13:YC:438[C]:LEU:CD2 | 2.42 | 0.50 |
| 13:YB:571[F]:ARG:HD3 | 13:YC:564[F]:GLN:HE22 | 1.77 | 0.50 |
| 13:YA:557[F]:MET:HG2 | 13:YC:565[F]:TYR:CZ | 2.47 | 0.50 |
| 13:YC:66[C]:MET:O | 13:YC:69[C]:ILE:N | 2.44 | 0.50 |
| 13:YC:66[D]:MET:O | 13:YC:69[D]:ILE:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:124[E]:PHE:CE2 | 14:YD:135[E]:MET:HE2 | 2.47 | 0.50 |
| 1:X:130:ARG:HD3 | 14:YD:181[B]:GLY:HA2 | 1.93 | 0.50 |
| 14:YD:278[A]:SER:O | 14:YD:279[A]:ARG:NH1 | 2.41 | 0.50 |
| 14:YD:296[A]:ILE:HD11 | 14:YD:367[A]:ILE:HA | 1.93 | 0.50 |
| 14:YD:92[E]:HIS:NE2 | 14:YF:238[E]:THR:OG1 | 2.44 | 0.50 |
| 14:YF:296[C]:ILE:HD11 | 14:YF:367[C]:ILE:HA | 1.93 | 0.50 |
| 2:Z:172:GLU:OE1 | 4:AA:164:ILE:HG23 | 81.71 | 0.50 |
| 15:ZA:31[B]:THR:OG1 | 15:ZA:94[B]:VAL:HG21 | 2.12 | 0.50 |
| 15:ZA:29[D]:VAL:HG21 | 15:ZA:69[D]:VAL:HG13 | 1.94 | 0.50 |
| 15:ZA:31[D]:THR:OG1 | 15:ZA:94[D]:VAL:HG21 | 2.12 | 0.50 |
| 1:A:318:ASP:HB3 | 1:A:319:PRO:C | 2.32 | 0.50 |
| 1:A:430:GLN:H | 1:A:430:GLN:CD | 2.14 | 0.50 |
| 1:A:512:SER:OG | 1:A:513:ASN:N | 2.44 | 0.50 |
| 5:AC:161:ASN:HB2 | 5:AC:248:MET:SD | 2.52 | 0.50 |
| 5:AC:322:GLY:C | 5:AC:359:GLU:HA | 2.32 | 0.50 |
| 5:AC:262:GLN:HG2 | 5:AC:382:ASN:HD22 | 1.76 | 0.50 |
| 5:AC:506:LEU:HB3 | 5:AC:510:GLY:HA2 | 1.93 | 0.50 |
| 5:AE:206:PHE:HZ | 5:AE:221:GLU:HG2 | 1.75 | 0.50 |
| 6:AF:122:ALA:O | 6:AF:126:VAL:HG23 | 2.12 | 0.50 |
| 6:AF:147:LYS:O | 6:AF:157:GLU:N | 2.44 | 0.50 |
| 5:AE:264:ARG:HH12 | 6:AF:2:SER:N | 2.10 | 0.50 |
| 7:AI:32:VAL:O | 7:AI:36:ILE:N | 2.39 | 0.50 |
| 7:AI:451:PHE:HD1 | 7:AI:469:VAL:HG13 | 1.75 | 0.50 |
| 1:B:153:ALA:HB2 | 1:B:163:PRO:HB3 | 1.93 | 0.50 |
| 1:B:424:TYR:OH | 1:B:657:PRO:HG3 | 2.11 | 0.50 |
| 1:B:526:PRO:HB2 | 1:B:528:THR:HG23 | 1.94 | 0.50 |
| 8:BB:137:VAL:HA | 8:BB:155:VAL:HG12 | 1.93 | 0.50 |
| 9:BD:105:ILE:HA | 9:BD:125:GLN:HA | 1.93 | 0.50 |
| 12:BG:220:SER:HA | 12:BG:243:PHE:CD1 | 2.47 | 0.50 |
| 1:BH:278:ALA:HA | 1:BH:316:GLY:HA3 | 1.94 | 0.50 |
| 1:BH:555:ILE:HG13 | 1:BH:556:GLY:N | 2.27 | 0.50 |
| 1:BH:566:ASN:HB3 | 1:BH:569:ILE:HG13 | 1.94 | 0.50 |
| 1:BI:219:SER:O | 1:BI:220:THR:OG1 | 2.29 | 0.50 |
| 1:BI:340:VAL:HG22 | 1:BI:341:THR:H | 1.76 | 0.50 |
| 2:BJ:1000:THR:HG23 | 5:CF:17:ASP:O | 2.12 | 0.50 |
| 2:C:18:ALA:HA | 2:C:102:THR:HB | 1.94 | 0.50 |
| 3:CA:51:GLU:HA | 3:CA:56:PHE:CD2 | 2.46 | 0.50 |
| 3:CA:63:ASP:HB2 | 3:CB:13:THR:HG23 | 1.93 | 0.50 |
| 3:CB:89:VAL:HG12 | 3:CB:209:VAL:HA | 1.94 | 0.50 |
| 3:CB:271:GLN:HB2 | 3:CB:313:GLU:O | 2.11 | 0.50 |
| 2:BJ:9:THR:HG21 | 3:CB:57:ALA:HB3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CC:39:TYR:CG | 4:CD:7:LYS:HD3 | 2.46 | 0.50 |
| 4:CC:201:LYS:NZ | 4:CE:218:GLU:OE1 | 2.33 | 0.50 |
| 5:CF:568:LYS:HA | 5:CG:550:VAL:O | 2.11 | 0.50 |
| 5:CG:168:LEU:HA | 5:CG:241:THR:HG22 | 1.94 | 0.50 |
| 5:CG:335:ASP:OD1 | 5:CG:335:ASP:N | 2.45 | 0.50 |
| 5:CG:290:SER:N | 5:CG:371:PHE:O | 2.45 | 0.50 |
| 5:CH:194:LYS:O | 5:CH:242:VAL:HA | 2.11 | 0.50 |
| 6:DA:4:LEU:HD23 | 6:DA:5:ASN:N | 2.27 | 0.50 |
| 6:DA:35:VAL:HG13 | 6:DA:58:ASP:HB2 | 1.93 | 0.50 |
| 7:DB:99:ARG:NH1 | 7:DB:105:GLU:OE2 | 2.32 | 0.50 |
| 7:DB:27:PRO:HA | 7:DB:29:ILE:HD11 | 1.92 | 0.50 |
| 7:DB:417:ASN:HB3 | 7:DB:421:GLY:HA2 | 1.94 | 0.50 |
| 7:DB:216:MET:SD | 7:DC:202:GLY:HA3 | 2.52 | 0.50 |
| 7:DC:340:THR:HG22 | 7:DC:341:ILE:HG12 | 1.93 | 0.50 |
| 7:DC:78:PRO:HB2 | 7:DD:69:GLY:HA2 | 1.93 | 0.50 |
| 10:DH:340:SER:O | 10:DH:341:THR:HG23 | 2.11 | 0.50 |
| 11:DI:2:LEU:O | 11:DI:4:THR:N | 2.45 | 0.50 |
| 12:DJ:217:THR:O | 12:DJ:246:ARG:N | 2.32 | 0.50 |
| 2:C:898:MET:HE1 | 3:E:315:ARG:HH12 | 1.76 | 0.50 |
| 3:E:69:THR:O | 3:E:73:THR:N | 2.45 | 0.50 |
| 1:EB:98:TYR:CE2 | 1:EB:100:PRO:HA | 2.47 | 0.50 |
| 2:EC:796:THR:HG22 | 2:EC:812:THR:O | 2.12 | 0.50 |
| 3:ED:117:ALA:O | 3:ED:121:ALA:N | 2.45 | 0.50 |
| 3:ED:225:TYR:CE2 | 3:ED:231:TRP:HB3 | 2.47 | 0.50 |
| 3:ED:50:ASN:HB2 | 3:ED:56:PHE:CE1 | 2.47 | 0.50 |
| 3:EE:89:VAL:HG12 | 3:EE:209:VAL:HA | 1.94 | 0.50 |
| 4:EF:139:VAL:HG21 | 4:EF:146:VAL:HG21 | 1.93 | 0.50 |
| 4:EH:201:LYS:NZ | 4:EH:220:ASN:OD1 | 2.37 | 0.50 |
| 5:EI:194:LYS:HB2 | 5:EI:243:GLN:HB2 | 1.92 | 0.50 |
| 5:EI:316:ILE:HD13 | 6:FD:7:LYS:HG3 | 1.94 | 0.50 |
| 5:EI:7:ILE:HG12 | 5:EJ:24:ILE:HG13 | 1.93 | 0.50 |
| 5:EJ:320:LEU:HG | 5:EJ:357:SER:CB | 2.42 | 0.50 |
| 6:FB:32:ARG:NH1 | 6:FC:144:ASN:OD1 | 2.43 | 0.50 |
| 6:FC:4:LEU:HD23 | 6:FC:5:ASN:N | 2.27 | 0.50 |
| 7:FE:211:SER:O | 7:FE:215:PHE:N | 2.43 | 0.50 |
| 7:FF:119:ALA:O | 7:FF:122:THR:OG1 | 2.24 | 0.50 |
| 7:FE:477:TRP:CZ3 | 7:FF:469:VAL:HB | 2.47 | 0.50 |
| 7:FG:123:VAL:O | 7:FG:127:ASN:N | 2.26 | 0.50 |
| 7:FG:367:VAL:O | 7:FG:389:ASN:HA | 2.12 | 0.50 |
| 7:FG:66:VAL:O | 7:FG:84:ARG:NH2 | 2.45 | 0.50 |
| 1:GD:116:ASP:HB2 | 1:GD:161:TYR:OH | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:555:ILE:HG13 | 1:GD:556:GLY:N | 2.27 | 0.50 |
| 1:GE:510:MET:SD | 1:GE:602:ILE:HD13 | 2.52 | 0.50 |
| 2:GF:191:TYR:CE1 | 2:GF:235:LYS:HA | 2.47 | 0.50 |
| 2:GF:58:ASN:OD1 | 2:GF:59:LEU:N | 2.44 | 0.50 |
| 2:GF:796:THR:HG22 | 2:GF:812:THR:O | 2.12 | 0.50 |
| 2:GF:968:ASP:HB3 | 2:GF:972:GLU:CG | 2.42 | 0.50 |
| 4:F:201:LYS:NZ | 4:H:218:GLU:OE1 | 2.34 | 0.50 |
| 4:HA:139:VAL:HG21 | 4:HA:146:VAL:HG21 | 1.93 | 0.50 |
| 5:HB:289:LYS:O | 5:HB:290:SER:OG | 2.24 | 0.50 |
| 5:HB:334:ALA:HA | 5:HB:349:TRP:CD1 | 2.47 | 0.50 |
| 6:HE:147:LYS:O | 6:HE:157:GLU:N | 2.44 | 0.50 |
| 7:HH:106:ALA:HB2 | 7:HH:120:LYS:HD2 | 1.94 | 0.50 |
| 7:HH:47:VAL:HG12 | 7:HH:48:PRO:N | 2.26 | 0.50 |
| 7:HJ:375:TYR:HE2 | 7:HJ:390:PRO:HB2 | 1.77 | 0.50 |
| 5:I:249:ASP:OD1 | 5:J:160:SER:HB2 | 2.12 | 0.50 |
| 5:K:490:TRP:CD1 | 5:K:516:ALA:HA | 2.46 | 0.50 |
| 6:L:4:LEU:HD23 | 6:L:5:ASN:N | 2.27 | 0.50 |
| 6:M:54:SER:O | 6:N:164:GLN:NE2 | 2.44 | 0.50 |
| 10:U:208:THR:HA | 10:U:345:GLU:HG2 | 1.94 | 0.50 |
| 13:YA:109[D]:ASN:HB3 | 13:YA:112[D]:GLU:HB2 | 1.94 | 0.50 |
| 13:YA:270[D]:ASN:O | 13:YA:274[D]:GLN:N | 2.42 | 0.50 |
| 13:YA:344[D]:LYS:HA | 13:YA:344[D]:LYS:HE2 | 1.93 | 0.50 |
| 13:YA:344[E]:LYS:HE2 | 13:YA:344[E]:LYS:HA | 1.93 | 0.50 |
| 13:YA:367[A]:PRO:HA | 13:YC:315[A]:LEU:HD23 | 1.94 | 0.50 |
| 13:YA:538[F]:VAL:HG21 | 13:YB:534[F]:LEU:HD22 | 1.94 | 0.50 |
| 13:YA:563[C]:GLY:N | 13:YB:555[C]:ALA:O | 2.45 | 0.50 |
| 13:YA:13[D]:GLY:O | 13:YA:82[D]:VAL:N | 2.45 | 0.50 |
| 13:YB:416[F]:HIS:CE1 | 13:YB:417[F]:PRO:HD2 | 2.47 | 0.50 |
| 13:YA:529[F]:THR:N | 13:YB:520[F]:THR:O | 2.44 | 0.50 |
| 13:YB:554[A]:MET:HA | 13:YC:546[A]:VAL:O | 2.11 | 0.50 |
| 13:YC:66[A]:MET:O | 13:YC:69[A]:ILE:N | 2.44 | 0.50 |
| 13:YC:57[F]:VAL:HB | 13:YC:76[F]:PRO:HD3 | 1.93 | 0.50 |
| 14:YD:47[E]:ARG:O | 14:YD:48[E]:ASN:ND2 | 2.45 | 0.50 |
| 10:U:285:LEU:HA | 14:YE:215[E]:GLU:HG3 | 1.94 | 0.50 |
| 14:YE:360[F]:ASN:ND2 | 14:YE:360[F]:ASN:H | 2.04 | 0.50 |
| 14:YE:296[A]:ILE:HD11 | 14:YE:367[A]:ILE:HA | 1.93 | 0.50 |
| 14:YE:373[D]:LYS:HG2 | 14:YE:374[D]:ASN:N | 2.26 | 0.50 |
| 14:YE:47[C]:ARG:O | 14:YE:48[C]:ASN:ND2 | 2.45 | 0.50 |
| 14:YF:278[B]:SER:O | 14:YF:279[B]:ARG:NH1 | 2.42 | 0.50 |
| 2:Z:253:ILE:HG13 | 2:Z:300:LEU:HD21 | 1.94 | 0.50 |
| 2:Z:316:ASP:HA | 2:Z:331:THR:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:ZA:67[C]:VAL:HG21 | 15:ZA:96[C]:ILE:HB | 1.92 | 0.50 |
| 15:ZA:29[C]:VAL:HG21 | 15:ZA:69[C]:VAL:HG13 | 1.94 | 0.50 |
| 1:A:566:ASN:HB3 | 1:A:569:ILE:HG13 | 1.94 | 0.50 |
| 4:AA:61:ILE:O | 4:AB:4:GLN:NE2 | 2.44 | 0.50 |
| 5:AC:200:LEU:HD11 | 5:AD:241:THR:HG21 | 1.94 | 0.50 |
| 5:AD:289:LYS:O | 5:AD:290:SER:OG | 2.25 | 0.50 |
| 6:AG:122:ALA:O | 6:AG:126:VAL:HG23 | 2.12 | 0.50 |
| 7:AI:140:GLY:O | 7:BA:141:VAL:HG23 | 2.12 | 0.50 |
| 7:AI:264:LYS:O | 7:AI:279:SER:HA | 2.11 | 0.50 |
| 7:AJ:14:ARG:HG2 | 7:AJ:33:GLN:HG2 | 1.93 | 0.50 |
| 7:AI:480:ARG:HD3 | 7:AJ:462:ASN:ND2 | 2.27 | 0.50 |
| 1:A:400:ASN:O | 1:B:341:THR:HA | 2.11 | 0.50 |
| 1:B:444:ILE:O | 1:B:447:TYR:N | 2.45 | 0.50 |
| 7:AI:346:ILE:N | 7:BA:348:MET:O | 2.28 | 0.50 |
| 1:BI:461:LYS:HE3 | 1:BI:630:ASP:OD1 | 2.12 | 0.50 |
| 2:BJ:253:ILE:HG13 | 2:BJ:300:LEU:HD21 | 1.94 | 0.50 |
| 2:BJ:408:HIS:HB3 | 2:BJ:410:GLU:CD | 2.31 | 0.50 |
| 2:BJ:796:THR:HG22 | 2:BJ:812:THR:O | 2.12 | 0.50 |
| 3:CB:144:ILE:HG22 | 3:CB:146:SER:H | 1.77 | 0.50 |
| 4:CE:30:LYS:O | 4:CE:34:ASP:N | 2.45 | 0.50 |
| 5:CF:170:GLU:HA | 5:CF:238:ILE:HG13 | 1.94 | 0.50 |
| 6:DA:149:HIS:HB3 | 6:DA:152:ASP:O | 2.11 | 0.50 |
| 7:DC:167:GLN:O | 7:DC:170:ILE:N | 2.45 | 0.50 |
| 7:DB:45:ASN:CG | 7:DC:24:ASN:HD21 | 2.15 | 0.50 |
| 7:DD:20:PRO:HD3 | 7:DD:29:ILE:HG21 | 1.92 | 0.50 |
| 7:DB:407:SER:N | 7:DD:394:ASP:OD2 | 2.38 | 0.50 |
| 1:EA:116:ASP:HB2 | 1:EA:161:TYR:OH | 2.12 | 0.50 |
| 1:EA:539:ARG:CD | 1:EA:580:LEU:HD23 | 2.41 | 0.50 |
| 2:EC:17:SER:HA | 2:EC:106:ASN:HB3 | 1.93 | 0.50 |
| 2:EC:58:ASN:OD1 | 2:EC:59:LEU:N | 2.44 | 0.50 |
| 2:EC:817:LEU:HD11 | 3:EE:252:TYR:CE2 | 2.46 | 0.50 |
| 2:EC:926:PRO:HG2 | 2:EC:985:GLU:HG2 | 1.94 | 0.50 |
| 3:ED:7:ILE:HD11 | 3:EE:316:PRO:HG2 | 1.94 | 0.50 |
| 3:EE:69:THR:O | 3:EE:73:THR:N | 2.45 | 0.50 |
| 4:EG:70:HIS:HB2 | 4:EG:75:TYR:CE2 | 2.47 | 0.50 |
| 5:EI:161:ASN:HB2 | 5:EI:248:MET:SD | 2.52 | 0.50 |
| 5:EI:200:LEU:HD11 | 5:EJ:241:THR:HG21 | 1.93 | 0.50 |
| 5:FA:200:LEU:HD23 | 5:FA:210:SER:HA | 1.93 | 0.50 |
| 5:FA:206:PHE:HZ | 5:FA:221:GLU:HG2 | 1.76 | 0.50 |
| 6:FB:4:LEU:HD23 | 6:FB:5:ASN:N | 2.27 | 0.50 |
| 5:FA:313:PHE:CE1 | 6:FC:8:ALA:HB1 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FD:4:LEU:HD23 | 6:FD:5:ASN:N | 2.27 | 0.50 |
| 7:FE:160:MET:SD | 7:FE:165:THR:HB | 2.52 | 0.50 |
| 7:FE:452:GLY:HA3 | 7:FG:480:ARG:O | 2.11 | 0.50 |
| 7:FF:167:GLN:O | 7:FF:170:ILE:N | 2.45 | 0.50 |
| 7:FF:77:THR:HG23 | 7:FF:79:ALA:H | 1.77 | 0.50 |
| 9:FJ:105:ILE:HA | 9:FJ:125:GLN:HA | 1.93 | 0.50 |
| 10:GA:132:SER:HA | 10:GA:209:TRP:NE1 | 2.25 | 0.50 |
| 10:GA:285:LEU:HA | 14:YE:215[C]:GLU:HG3 | 1.93 | 0.50 |
| 10:GA:332:LEU:HD21 | 10:GA:340:SER:CB | 2.41 | 0.50 |
| 11:GB:2:LEU:O | 11:GB:4:THR:N | 2.45 | 0.50 |
| 12:GC:159:VAL:HG22 | 12:GC:242:THR:HG22 | 1.93 | 0.50 |
| 1:GD:111:MET:SD | 1:GD:304:PRO:HB3 | 2.52 | 0.50 |
| 2:GF:1014:ASP:CG | 2:GF:1015:ASN:H | 2.15 | 0.50 |
| 3:GG:216:LEU:HD23 | 3:GG:236:PHE:HB3 | 1.93 | 0.50 |
| 4:H:193:HIS:HA | 4:H:260:TYR:HD1 | 1.77 | 0.50 |
| 5:HB:454:TYR:CD1 | 5:HB:458:THR:HG21 | 2.47 | 0.50 |
| 5:HB:1:MET:N | 5:HC:41:ASP:HB3 | 2.26 | 0.50 |
| 2:GF:221:ALA:O | 5:HC:564:PRO:HG2 | 2.12 | 0.50 |
| 5:HD:501:LEU:HB3 | 5:HD:512:PRO:HB2 | 1.94 | 0.50 |
| 6:HE:122:ALA:O | 6:HE:126:VAL:HG23 | 2.12 | 0.50 |
| 6:HG:73:ASN:HD21 | 6:HG:215:PHE:HE2 | 1.60 | 0.50 |
| 7:HI:221:THR:HG23 | 7:HI:224:TYR:H | 1.77 | 0.50 |
| 5:I:182:ARG:NH2 | 5:J:299:ILE:HG21 | 2.27 | 0.50 |
| 11:IE:147:GLU:OE1 | 11:IE:147:GLU:N | 2.45 | 0.50 |
| 12:IF:156:ASP:OD1 | 12:IF:157:PRO:HD2 | 2.12 | 0.50 |
| 5:J:159:ILE:HG23 | 5:J:246:THR:HG21 | 1.94 | 0.50 |
| 5:J:261:ARG:NE | 5:J:297:GLY:O | 2.30 | 0.50 |
| 5:K:477:SER:N | 5:K:602:ALA:O | 2.28 | 0.50 |
| 6:L:149:HIS:HB3 | 6:L:152:ASP:O | 2.11 | 0.50 |
| 6:L:82:VAL:HB | 6:L:187:LYS:HB3 | 1.92 | 0.50 |
| 6:L:200:THR:OG1 | 6:M:204:ASP:OD2 | 2.30 | 0.50 |
| 6:N:149:HIS:HB3 | 6:N:152:ASP:O | 2.11 | 0.50 |
| 7:P:221:THR:HG23 | 7:P:224:TYR:H | 1.77 | 0.50 |
| 7:O:308:ILE:HD11 | 7:Q:306:PHE:HB3 | 1.93 | 0.50 |
| 8:R:139:GLU:H | 8:IA:43:ALA:HB2 | 1.77 | 0.50 |
| 12:W:159:VAL:HG22 | 12:W:242:THR:HG22 | 1.93 | 0.50 |
| 1:X:318:ASP:HB3 | 1:X:319:PRO:C | 2.32 | 0.50 |
| 1:X:460:ALA:HA | 1:X:631:VAL:HG12 | 1.93 | 0.50 |
| 1:X:543:THR:OG1 | 1:X:544:ASP:N | 2.45 | 0.50 |
| 13:YA:416[D]:HIS:CE1 | 13:YA:417[D]:PRO:HD2 | 2.47 | 0.50 |
| 13:YA:416[E]:HIS:CE1 | 13:YA:417[E]:PRO:HD2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:416[B]:HIS:CE1 | 13:YA:417[B]:PRO:HD2 | 2.47 | 0.50 |
| 13:YA:428[B]:GLY:HA3 | 13:YC:418[B]:THR:HG21 | 1.93 | 0.50 |
| 13:YA:436[E]:ASP:OD2 | 13:YA:437[E]:ASN:N | 2.45 | 0.50 |
| 13:YA:490[C]:VAL:O | 13:YC:498[C]:VAL:HA | 2.11 | 0.50 |
| 13:YA:66[D]:MET:O | 13:YA:69[D]:ILE:N | 2.44 | 0.50 |
| 13:YA:13[F]:GLY:O | 13:YA:82[F]:VAL:N | 2.45 | 0.50 |
| 13:YA:9[C]:ASN:HA | 13:YC:7[C]:ASN:ND2 | 2.17 | 0.50 |
| 13:YA:71[B]:GLY:HA2 | 13:YB:393[B]:MET:HA | 1.92 | 0.50 |
| 13:YB:416[A]:HIS:CE1 | 13:YB:417[A]:PRO:HD2 | 2.47 | 0.50 |
| 13:YB:416[C]:HIS:CE1 | 13:YB:417[C]:PRO:HD2 | 2.47 | 0.50 |
| 13:YB:379[D]:PRO:HG2 | 13:YB:429[D]:ARG:CZ | 2.41 | 0.50 |
| 13:YB:485[C]:ASP:O | 13:YC:478[C]:ASN:N | 2.45 | 0.50 |
| 13:YB:554[D]:MET:HA | 13:YC:546[D]:VAL:O | 2.11 | 0.50 |
| 13:YC:266[D]:TRP:O | 13:YC:274[D]:GLN:NE2 | 2.45 | 0.50 |
| 13:YC:344[D]:LYS:HE2 | 13:YC:344[D]:LYS:HA | 1.93 | 0.50 |
| 13:YB:442[B]:THR:HG21 | 13:YC:438[B]:LEU:CD2 | 2.42 | 0.50 |
| 13:YB:503[C]:THR:O | 13:YC:495[C]:THR:HA | 2.10 | 0.50 |
| 13:YB:571[B]:ARG:HD3 | 13:YC:564[B]:GLN:HE22 | 1.77 | 0.50 |
| 13:YA:557[C]:MET:HG2 | 13:YC:565[C]:TYR:CZ | 2.47 | 0.50 |
| 13:YC:13[D]:GLY:O | 13:YC:82[D]:VAL:N | 2.45 | 0.50 |
| 14:YD:101[D]:GLY:HA2 | 14:YF:332[D]:GLN:OE1 | 2.12 | 0.50 |
| 14:YD:278[C]:SER:O | 14:YD:279[C]:ARG:NH1 | 2.44 | 0.50 |
| 14:YD:332[B]:GLN:OE1 | 14:YE:101[B]:GLY:HA2 | 2.12 | 0.50 |
| 14:YE:278[C]:SER:O | 14:YE:279[C]:ARG:NH1 | 2.44 | 0.50 |
| 14:YE:332[D]:GLN:OE1 | 14:YF:101[D]:GLY:HA2 | 2.11 | 0.50 |
| 2:Z:231:TYR:HE2 | 2:Z:389:ASN:HD21 | 1.58 | 0.50 |
| 2:Z:514:PHE:CD1 | 2:Z:525:TRP:HB2 | 2.45 | 0.50 |
| 15:ZA:31[C]:THR:OG1 | 15:ZA:94[C]:VAL:HG21 | 2.12 | 0.50 |
| 15:ZA:31[F]:THR:OG1 | 15:ZA:94[F]:VAL:HG21 | 2.12 | 0.50 |
| 15:ZA:29[B]:VAL:HG21 | 15:ZA:69[B]:VAL:HG13 | 1.94 | 0.50 |
| 15:ZA:67[E]:VAL:HG21 | 15:ZA:96[E]:ILE:HB | 1.92 | 0.50 |
| 1:A:111:MET:SD | 1:A:304:PRO:HB3 | 2.52 | 0.50 |
| 4:AB:79:VAL:N | 4:AB:97:ILE:O | 2.31 | 0.50 |
| 5:AC:359:GLU:H | 5:AC:370:HIS:C | 2.15 | 0.50 |
| 5:AE:194:LYS:O | 5:AE:242:VAL:HA | 2.11 | 0.50 |
| 7:AI:160:MET:SD | 7:AI:165:THR:HB | 2.52 | 0.50 |
| 7:AI:246:THR:HG1 | 7:AI:249:THR:H | 1.59 | 0.50 |
| 1:B:105:ALA:HB2 | 1:B:275:THR:HG21 | 1.92 | 0.50 |
| 7:BA:367:VAL:O | 7:BA:389:ASN:HA | 2.12 | 0.50 |
| 8:BC:143:ASP:OD1 | 8:BC:144:TRP:N | 2.45 | 0.50 |
| 10:BE:222:ILE:O | 10:BE:225:ILE:HG22 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:BG:156:ASP:OD1 | 12:BG:157:PRO:HD2 | 2.12 | 0.50 |
| 1:BH:636:ASP:N | 1:BH:636:ASP:OD1 | 2.44 | 0.50 |
| 2:BJ:316:ASP:HA | 2:BJ:331:THR:O | 2.11 | 0.50 |
| 2:C:916:TYR:HB3 | 2:C:1004:PHE:HB3 | 1.94 | 0.50 |
| 2:C:173:TYR:CE1 | 2:C:579:LYS:HE2 | 2.47 | 0.50 |
| 2:C:817:LEU:HD11 | 3:E:252:TYR:CE2 | 2.47 | 0.50 |
| 3:CA:117:ALA:O | 3:CA:121:ALA:N | 2.45 | 0.50 |
| 4:CD:204:VAL:HG22 | 4:CD:276:VAL:HG22 | 1.92 | 0.50 |
| 4:CD:113:ASN:ND2 | 4:CE:103:LEU:HD21 | 2.19 | 0.50 |
| 5:CF:67:SER:CB | 5:CF:94:ARG:HB2 | 2.42 | 0.50 |
| 5:CG:320:LEU:HG | 5:CG:357:SER:CB | 2.42 | 0.50 |
| 5:CH:252:SER:O | 5:CH:255:ARG:HB2 | 2.12 | 0.50 |
| 5:CH:395:THR:HG22 | 5:CH:396:LYS:H | 1.77 | 0.50 |
| 6:CJ:122:ALA:O | 6:CJ:126:VAL:HG23 | 2.12 | 0.50 |
| 7:DC:77:THR:HG23 | 7:DC:79:ALA:H | 1.77 | 0.50 |
| 7:DB:441:GLN:N | 7:DD:513:ARG:O | 2.35 | 0.50 |
| 10:DH:313:PRO:HG2 | 10:DH:351:ILE:HG22 | 1.93 | 0.50 |
| 3:E:72:TRP:NE1 | 3:E:304:ARG:HD3 | 2.27 | 0.50 |
| 1:EA:111:MET:SD | 1:EA:304:PRO:HB3 | 2.52 | 0.50 |
| 1:EA:318:ASP:HB3 | 1:EA:319:PRO:C | 2.32 | 0.50 |
| 1:EB:80:MET:HG3 | 1:EB:81:ARG:HG3 | 1.94 | 0.50 |
| 2:EC:357:ILE:HG12 | 2:EC:358:THR:H | 1.77 | 0.50 |
| 3:EE:61:PRO:HG3 | 3:EE:314:ASN:OD1 | 2.12 | 0.50 |
| 4:EG:193:HIS:HA | 4:EG:260:TYR:HD1 | 1.77 | 0.50 |
| 5:EI:170:GLU:HA | 5:EI:238:ILE:HG13 | 1.94 | 0.50 |
| 5:EI:201:TYR:HB3 | 5:EJ:166:GLU:HG2 | 1.93 | 0.50 |
| 5:EI:359:GLU:H | 5:EI:370:HIS:C | 2.15 | 0.50 |
| 5:EJ:147:LYS:HE2 | 5:EJ:155:THR:HB | 1.94 | 0.50 |
| 5:EJ:415:ASP:HB2 | 5:EJ:440:GLN:HE22 | 1.76 | 0.50 |
| 5:FA:138:CYS:SG | 5:FA:140:PRO:HD2 | 2.51 | 0.50 |
| 5:FA:87:ASN:HA | 5:FA:89:TYR:CE2 | 2.47 | 0.50 |
| 6:FB:73:ASN:HD21 | 6:FB:215:PHE:HE2 | 1.60 | 0.50 |
| 7:FE:315:ILE:HG12 | 7:FG:308:ILE:HD12 | 1.94 | 0.50 |
| 7:FF:14:ARG:HG2 | 7:FF:33:GLN:HG2 | 1.93 | 0.50 |
| 7:FE:482:TYR:OH | 7:FF:453:GLU:HB2 | 2.11 | 0.50 |
| 4:G:107:VAL:O | 4:G:148:LEU:N | 2.39 | 0.50 |
| 4:G:53:GLY:HA3 | 4:H:7:LYS:HE2 | 1.94 | 0.50 |
| 10:GA:208:THR:HA | 10:GA:345:GLU:HG2 | 1.94 | 0.50 |
| 1:GE:187:ILE:HD11 | 1:GE:270:ILE:HD13 | 1.93 | 0.50 |
| 1:GE:461:LYS:HE3 | 1:GE:630:ASP:OD1 | 2.12 | 0.50 |
| 2:GF:193:MET:HG3 | 2:GF:238:TYR:CZ | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:89:VAL:HG12 | 3:GH:209:VAL:HA | 1.94 | 0.50 |
| 3:GH:69:THR:O | 3:GH:73:THR:N | 2.45 | 0.50 |
| 4:GJ:30:LYS:O | 4:GJ:34:ASP:N | 2.45 | 0.50 |
| 4:GJ:53:GLY:O | 4:HA:7:LYS:HB3 | 2.12 | 0.50 |
| 5:HB:161:ASN:HB2 | 5:HB:248:MET:SD | 2.52 | 0.50 |
| 5:HD:206:PHE:HZ | 5:HD:221:GLU:HG2 | 1.76 | 0.50 |
| 5:HD:192:ARG:HG3 | 5:HD:245:GLU:HB2 | 1.93 | 0.50 |
| 5:HD:340:VAL:HG21 | 6:HE:174:TYR:H | 1.76 | 0.50 |
| 7:HH:140:GLY:O | 7:HJ:141:VAL:HG23 | 2.12 | 0.50 |
| 5:I:149:LYS:HG2 | 5:I:150:GLN:N | 2.27 | 0.50 |
| 5:I:268:SER:N | 5:I:283:THR:O | 2.35 | 0.50 |
| 5:I:334:ALA:HA | 5:I:349:TRP:CD1 | 2.47 | 0.50 |
| 5:I:67:SER:CB | 5:I:94:ARG:HB2 | 2.42 | 0.50 |
| 8:IA:143:ASP:OD1 | 8:IA:144:TRP:N | 2.45 | 0.50 |
| 11:IE:178:ASN:HB3 | 14:YD:217[F]:SER:H | 1.77 | 0.50 |
| 5:K:200:LEU:HD23 | 5:K:210:SER:HA | 1.93 | 0.50 |
| 2:C:995:ASP:HB2 | 5:K:7:ILE:HG22 | 1.93 | 0.50 |
| 6:L:122:ALA:O | 6:L:126:VAL:HG23 | 2.12 | 0.50 |
| 6:M:149:HIS:HB3 | 6:M:152:ASP:O | 2.11 | 0.50 |
| 6:N:122:ALA:O | 6:N:126:VAL:HG23 | 2.12 | 0.50 |
| 7:Q:375:TYR:HE2 | 7:Q:390:PRO:HB2 | 1.77 | 0.50 |
| 8:S:143:ASP:OD1 | 8:S:144:TRP:N | 2.45 | 0.50 |
| 8:S:31:ASN:HB3 | 1:Y:76:TYR:CE1 | 191.47 | 0.50 |
| 11:V:178:ASN:H | 14:YD:217[A]:SER:C | 2.15 | 0.50 |
| 1:Y:19:GLU:HG2 | 1:Y:19:GLU:O | 2.12 | 0.50 |
| 13:YA:538[D]:VAL:HG21 | 13:YB:534[D]:LEU:HD22 | 1.94 | 0.50 |
| 13:YB:344[A]:LYS:HA | 13:YB:344[A]:LYS:HE2 | 1.93 | 0.50 |
| 13:YA:441[A]:ILE:HG21 | 13:YB:378[A]:GLU:OE2 | 2.11 | 0.50 |
| 13:YB:571[C]:ARG:HB3 | 13:YC:564[C]:GLN:NE2 | 2.26 | 0.50 |
| 13:YC:109[B]:ASN:HB3 | 13:YC:112[B]:GLU:HB2 | 1.93 | 0.50 |
| 13:YC:270[C]:ASN:O | 13:YC:274[C]:GLN:N | 2.42 | 0.50 |
| 13:YC:266[C]:TRP:O | 13:YC:274[C]:GLN:NE2 | 2.45 | 0.50 |
| 13:YA:428[D]:GLY:HA3 | 13:YC:418[D]:THR:HG21 | 1.93 | 0.50 |
| 13:YB:538[C]:VAL:HA | 13:YC:530[C]:VAL:O | 2.12 | 0.50 |
| 13:YB:571[E]:ARG:HD3 | 13:YC:564[E]:GLN:HE22 | 1.77 | 0.50 |
| 13:YA:557[E]:MET:HG2 | 13:YC:565[E]:TYR:CZ | 2.47 | 0.50 |
| 13:YC:66[E]:MET:O | 13:YC:69[E]:ILE:N | 2.45 | 0.50 |
| 14:YD:373[F]:LYS:HG2 | 14:YD:374[F]:ASN:N | 2.27 | 0.50 |
| 14:YD:97[E]:VAL:HG21 | 14:YF:332[E]:GLN:NE2 | 2.27 | 0.50 |
| 14:YE:45[A]:TYR:O | 14:YE:174[A]:ARG:NH2 | 2.45 | 0.50 |
| 14:YE:45[E]:TYR:O | 14:YE:174[E]:ARG:NH2 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:V:190:LYS:HZ1 | 14:YE:24[F]:SER:HA | 1.77 | 0.50 |
| 14:YE:293[F]:GLU:N | 14:YE:293[F]:GLU:OE1 | 2.45 | 0.50 |
| 14:YE:296[E]:ILE:HD11 | 14:YE:367[E]:ILE:HA | 1.94 | 0.50 |
| 14:YF:124[D]:PHE:CE2 | 14:YF:135[D]:MET:HE2 | 2.47 | 0.50 |
| 14:YF:373[B]:LYS:HG2 | 14:YF:374[B]:ASN:N | 2.26 | 0.50 |
| 14:YF:373[E]:LYS:HG2 | 14:YF:374[E]:ASN:N | 2.26 | 0.50 |
| 2:Z:1014:ASP:CG | 2:Z:1015:ASN:H | 2.15 | 0.50 |
| 2:Z:408:HIS:HB3 | 2:Z:410:GLU:CD | 2.31 | 0.50 |
| 15:ZA:31[A]:THR:OG1 | 15:ZA:94[A]:VAL:HG21 | 2.12 | 0.50 |
| 5:AC:94:ARG:HD3 | 5:AC:134:GLU:HG2 | 1.93 | 0.49 |
| 5:AC:1:MET:N | 5:AD:41:ASP:HB3 | 2.27 | 0.49 |
| 5:AC:67:SER:CB | 5:AC:94:ARG:HB2 | 2.42 | 0.49 |
| 5:AE:206:PHE:CG | 5:AE:223:VAL:HA | 2.47 | 0.49 |
| 5:AE:252:SER:O | 5:AE:255:ARG:HB2 | 2.12 | 0.49 |
| 5:AD:472:TYR:HA | 5:AE:416:ILE:HG23 | 1.93 | 0.49 |
| 7:AI:106:ALA:HB2 | 7:AI:120:LYS:HD2 | 1.94 | 0.49 |
| 7:BA:66:VAL:O | 7:BA:84:ARG:NH2 | 2.45 | 0.49 |
| 11:BF:138:ASP:HB3 | 11:BF:140:ALA:H | 1.77 | 0.49 |
| 2:C:336:ILE:O | 2:C:348:ARG:HB2 | 2.12 | 0.49 |
| 2:C:405:VAL:N | 2:C:414:LYS:O | 2.41 | 0.49 |
| 2:C:453:ASP:HB3 | 2:C:474:GLU:O | 2.12 | 0.49 |
| 3:CA:23:ASN:OD1 | 3:CB:27:SER:OG | 2.17 | 0.49 |
| 3:CA:92:ARG:NH1 | 3:CA:94:ASP:OD2 | 2.44 | 0.49 |
| 4:CD:70:HIS:HB2 | 4:CD:75:TYR:CE2 | 2.47 | 0.49 |
| 5:CF:334:ALA:HA | 5:CF:349:TRP:CD1 | 2.47 | 0.49 |
| 5:CH:138:CYS:SG | 5:CH:140:PRO:HD2 | 2.52 | 0.49 |
| 5:CH:558:ASP:OD1 | 5:CH:558:ASP:N | 2.45 | 0.49 |
| 6:CJ:4:LEU:HD23 | 6:CJ:5:ASN:N | 2.27 | 0.49 |
| 7:DB:140:GLY:O | 7:DD:141:VAL:HG23 | 2.12 | 0.49 |
| 7:DB:160:MET:SD | 7:DB:165:THR:HB | 2.51 | 0.49 |
| 7:DD:129:PHE:O | 7:DD:141:VAL:HG11 | 2.11 | 0.49 |
| 7:DD:361:PHE:HA | 7:DD:522:ILE:HA | 1.93 | 0.49 |
| 7:DB:84:ARG:NH1 | 7:DD:85:LEU:HD22 | 2.27 | 0.49 |
| 11:DI:142:LYS:HB3 | 11:DI:143:TYR:CD2 | 2.45 | 0.49 |
| 12:DJ:30:PRO:HG2 | 12:DJ:177:TRP:NE1 | 2.27 | 0.49 |
| 12:BG:215:MET:HE1 | 12:DJ:99:SER:HB2 | 1.93 | 0.49 |
| 1:EA:339:CYS:HA | 1:EA:344:ASP:OD2 | 2.13 | 0.49 |
| 1:EB:185:ILE:O | 1:EB:235:GLU:HG2 | 2.12 | 0.49 |
| 1:EB:510:MET:SD | 1:EB:602:ILE:HD13 | 2.52 | 0.49 |
| 1:EB:627:PRO:HG3 | 1:EB:632:ILE:HD11 | 1.94 | 0.49 |
| 2:EC:321:VAL:HB | 2:EC:326:VAL:HG12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:319:TYR:CD1 | 2:EC:328:TYR:HB2 | 2.47 | 0.49 |
| 2:EC:339:ASP:HB3 | 2:EC:340:PRO:CD | 2.36 | 0.49 |
| 3:ED:226:GLU:OE1 | 3:ED:226:GLU:N | 2.34 | 0.49 |
| 2:BJ:449:LYS:HD2 | 3:ED:74:HIS:CE1 | 2.46 | 0.49 |
| 5:EI:322:GLY:C | 5:EI:359:GLU:HA | 2.32 | 0.49 |
| 5:EI:506:LEU:HB3 | 5:EI:510:GLY:HA2 | 1.93 | 0.49 |
| 5:EI:563:GLY:HA3 | 5:EI:566:TYR:OH | 2.12 | 0.49 |
| 5:EJ:206:PHE:CD2 | 5:EJ:223:VAL:HA | 2.47 | 0.49 |
| 6:FD:73:ASN:HD21 | 6:FD:215:PHE:HE2 | 1.59 | 0.49 |
| 7:FF:146:SER:HA | 7:FF:164:LYS:HZ3 | 1.77 | 0.49 |
| 7:FE:42:ALA:HB3 | 7:FG:43:GLY:O | 2.12 | 0.49 |
| 12:GC:156:ASP:OD1 | 12:GC:157:PRO:HD2 | 2.12 | 0.49 |
| 1:GD:318:ASP:HB3 | 1:GD:319:PRO:C | 2.32 | 0.49 |
| 1:GD:539:ARG:CD | 1:GD:580:LEU:HD23 | 2.42 | 0.49 |
| 1:GE:106:ALA:HB2 | 1:GE:280:ALA:HB1 | 1.93 | 0.49 |
| 2:GF:221:ALA:H | 5:HC:562:SER:CB | 2.24 | 0.49 |
| 2:GF:321:VAL:HB | 2:GF:326:VAL:HG12 | 1.94 | 0.49 |
| 2:GF:453:ASP:HB3 | 2:GF:474:GLU:O | 2.12 | 0.49 |
| 3:GH:92:ARG:HD3 | 3:GH:205:ASN:O | 2.11 | 0.49 |
| 4:GI:139:VAL:HG21 | 4:GI:146:VAL:HG21 | 1.94 | 0.49 |
| 4:GI:70:HIS:HB2 | 4:GI:75:TYR:CE2 | 2.47 | 0.49 |
| 4:HA:201:LYS:NZ | 4:HA:220:ASN:OD1 | 2.37 | 0.49 |
| 5:HB:568:LYS:HA | 5:HC:550:VAL:O | 2.12 | 0.49 |
| 5:HC:159:ILE:HG23 | 5:HC:246:THR:HG21 | 1.94 | 0.49 |
| 5:HC:590:GLN:OE1 | 5:HD:589:ILE:HA | 2.11 | 0.49 |
| 5:HB:339:GLU:HB3 | 6:HF:172:SER:O | 2.12 | 0.49 |
| 7:HH:235:GLU:OE1 | 7:HH:243:VAL:HG11 | 2.12 | 0.49 |
| 7:HI:167:GLN:O | 7:HI:170:ILE:N | 2.45 | 0.49 |
| 7:HI:228:ILE:H | 7:HJ:226:GLY:H | 1.60 | 0.49 |
| 7:HI:295:ILE:HG12 | 7:HJ:301:ARG:HD3 | 1.93 | 0.49 |
| 7:HH:260:ARG:HA | 7:HJ:263:VAL:O | 2.12 | 0.49 |
| 7:HJ:367:VAL:O | 7:HJ:389:ASN:HA | 2.12 | 0.49 |
| 5:I:289:LYS:O | 5:I:290:SER:OG | 2.24 | 0.49 |
| 8:IB:130:LYS:NZ | 8:IB:163:GLU:OE2 | 2.37 | 0.49 |
| 1:GE:76:TYR:CE1 | 11:IE:31:ASN:HB3 | 2.47 | 0.49 |
| 5:J:247:PHE:HZ | 5:K:162:VAL:HG21 | 1.77 | 0.49 |
| 5:J:290:SER:N | 5:J:371:PHE:O | 2.45 | 0.49 |
| 5:K:252:SER:O | 5:K:255:ARG:HB2 | 2.12 | 0.49 |
| 6:M:35:VAL:HG13 | 6:M:58:ASP:HB2 | 1.93 | 0.49 |
| 7:O:100:TYR:CZ | 7:P:113:GLU:HA | 2.46 | 0.49 |
| 7:O:42:ALA:HB3 | 7:Q:43:GLY:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:295:ILE:HG12 | 7:Q:301:ARG:HD3 | 1.93 | 0.49 |
| 5:K:196:ARG:NE | 7:P:5:THR:HG23 | 2.26 | 0.49 |
| 7:Q:386:ASN:HB2 | 7:Q:387:PRO:HD2 | 1.94 | 0.49 |
| 8:S:137:VAL:HA | 8:S:155:VAL:HG12 | 1.93 | 0.49 |
| 12:W:156:ASP:OD1 | 12:W:157:PRO:HD2 | 2.12 | 0.49 |
| 1:X:645:ASP:N | 1:X:645:ASP:OD1 | 2.45 | 0.49 |
| 1:X:647:ARG:HH11 | 1:X:650:TYR:HE2 | 1.60 | 0.49 |
| 1:Y:378:PRO:HG3 | 1:Y:384:LEU:HA | 1.93 | 0.49 |
| 13:YA:81[E]:ARG:HB3 | 13:YA:100[E]:TYR:CZ | 2.47 | 0.49 |
| 13:YA:266[C]:TRP:O | 13:YA:274[C]:GLN:NE2 | 2.45 | 0.49 |
| 13:YA:344[A]:LYS:HE2 | 13:YA:344[A]:LYS:HA | 1.93 | 0.49 |
| 13:YA:473[C]:GLN:HA | 13:YC:481[C]:PHE:O | 2.12 | 0.49 |
| 13:YA:474[D]:ILE:HG12 | 13:YB:466[D]:ASN:HB2 | 1.93 | 0.49 |
| 13:YA:474[E]:ILE:HG12 | 13:YB:466[E]:ASN:HB2 | 1.93 | 0.49 |
| 13:YA:563[D]:GLY:N | 13:YB:555[D]:ALA:O | 2.45 | 0.49 |
| 13:YA:57[F]:VAL:HB | 13:YA:76[F]:PRO:HD3 | 1.93 | 0.49 |
| 13:YB:16[E]:GLU:CD | 13:YB:30[E]:ARG:HH11 | 2.16 | 0.49 |
| 13:YB:344[B]:LYS:HE2 | 13:YB:344[B]:LYS:HA | 1.93 | 0.49 |
| 13:YB:416[E]:HIS:CE1 | 13:YB:417[E]:PRO:HD2 | 2.47 | 0.49 |
| 13:YB:485[B]:ASP:O | 13:YC:478[B]:ASN:N | 2.45 | 0.49 |
| 13:YB:522[C]:VAL:HG11 | 13:YB:526[C]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:538[B]:VAL:HG21 | 13:YB:534[B]:LEU:HD22 | 1.94 | 0.49 |
| 13:YC:266[A]:TRP:O | 13:YC:274[A]:GLN:NE2 | 2.45 | 0.49 |
| 13:YC:416[A]:HIS:CE1 | 13:YC:417[A]:PRO:HD2 | 2.47 | 0.49 |
| 13:YC:416[C]:HIS:CE1 | 13:YC:417[C]:PRO:HD2 | 2.47 | 0.49 |
| 13:YC:416[D]:HIS:CE1 | 13:YC:417[D]:PRO:HD2 | 2.47 | 0.49 |
| 13:YB:571[F]:ARG:HB3 | 13:YC:564[F]:GLN:NE2 | 2.26 | 0.49 |
| 13:YA:123[E]:ARG:HB2 | 13:YC:67[E]:SER:HB3 | 1.94 | 0.49 |
| 14:YD:45[A]:TYR:O | 14:YD:174[A]:ARG:NH2 | 2.45 | 0.49 |
| 14:YD:45[E]:TYR:O | 14:YD:174[E]:ARG:NH2 | 2.45 | 0.49 |
| 1:GD:130:ARG:HD3 | 14:YD:181[F]:GLY:HA2 | 1.92 | 0.49 |
| 14:YD:293[A]:GLU:N | 14:YD:293[A]:GLU:OE1 | 2.45 | 0.49 |
| 14:YD:296[D]:ILE:HD11 | 14:YD:367[D]:ILE:HA | 1.93 | 0.49 |
| 14:YD:373[D]:LYS:HG2 | 14:YD:374[D]:ASN:N | 2.26 | 0.49 |
| 14:YD:373[C]:LYS:HG2 | 14:YD:374[C]:ASN:N | 2.26 | 0.49 |
| 14:YD:45[B]:TYR:O | 14:YD:174[B]:ARG:NH2 | 2.45 | 0.49 |
| 14:YE:45[F]:TYR:O | 14:YE:174[F]:ARG:NH2 | 2.45 | 0.49 |
| 14:YE:293[D]:GLU:OE1 | 14:YE:293[D]:GLU:N | 2.44 | 0.49 |
| 14:YE:373[A]:LYS:HG2 | 14:YE:374[A]:ASN:N | 2.27 | 0.49 |
| 14:YE:47[D]:ARG:O | 14:YE:48[D]:ASN:ND2 | 2.45 | 0.49 |
| 14:YF:45[A]:TYR:O | 14:YF:174[A]:ARG:NH2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:45[E]:TYR:O | 14:YF:174[E]:ARG:NH2 | 2.45 | 0.49 |
| 1:A:344:ASP:O | 1:A:347:THR:N | 2.44 | 0.49 |
| 1:A:636:ASP:OD1 | 1:A:636:ASP:N | 2.44 | 0.49 |
| 5:AC:194:LYS:O | 5:AC:242:VAL:HA | 2.12 | 0.49 |
| 5:AD:419:ASP:OD1 | 5:AD:420:VAL:N | 2.45 | 0.49 |
| 7:AI:90:ALA:HB2 | 7:AI:96:GLY:CA | 2.42 | 0.49 |
| 7:AJ:221:THR:HG23 | 7:AJ:224:TYR:H | 1.77 | 0.49 |
| 1:B:106:ALA:HB2 | 1:B:280:ALA:HB1 | 1.93 | 0.49 |
| 1:B:187:ILE:HD11 | 1:B:270:ILE:HD13 | 1.93 | 0.49 |
| 1:B:518:ASN:OD1 | 1:B:535:LEU:HB3 | 2.12 | 0.49 |
| 7:BA:125:LEU:O | 7:BA:129:PHE:N | 2.40 | 0.49 |
| 7:AI:308:ILE:HD11 | 7:BA:306:PHE:HB3 | 1.94 | 0.49 |
| 7:BA:361:PHE:HA | 7:BA:522:ILE:HA | 1.93 | 0.49 |
| 12:BG:159:VAL:HG22 | 12:BG:242:THR:HG22 | 1.93 | 0.49 |
| 1:BH:318:ASP:HB3 | 1:BH:319:PRO:C | 2.32 | 0.49 |
| 1:BI:189:ASP:HA | 11:DI:121:TYR:CE2 | 2.47 | 0.49 |
| 2:BJ:682:GLN:O | 2:BJ:685:ASN:HB3 | 2.12 | 0.49 |
| 2:C:796:THR:HG22 | 2:C:812:THR:O | 2.12 | 0.49 |
| 3:CA:193:GLU:O | 3:CA:223:TRP:HA | 2.11 | 0.49 |
| 5:CF:322:GLY:C | 5:CF:359:GLU:HA | 2.32 | 0.49 |
| 5:CF:76:ARG:NH2 | 5:CF:78:THR:OG1 | 2.45 | 0.49 |
| 5:CG:267:ASP:OD1 | 5:CG:285:LEU:HB2 | 2.12 | 0.49 |
| 5:CH:490:TRP:CD1 | 5:CH:516:ALA:HA | 2.46 | 0.49 |
| 5:CF:569:TYR:CE2 | 5:CH:542:LEU:HD11 | 2.47 | 0.49 |
| 6:DA:122:ALA:O | 6:DA:126:VAL:HG23 | 2.12 | 0.49 |
| 6:DA:73:ASN:HD21 | 6:DA:215:PHE:HE2 | 1.60 | 0.49 |
| 7:DB:289:GLN:HB2 | 7:DC:286:ASP:O | 2.12 | 0.49 |
| 7:DB:480:ARG:HD3 | 7:DC:462:ASN:ND2 | 2.27 | 0.49 |
| 7:DB:138:SER:C | 7:DD:143:LYS:HG2 | 2.33 | 0.49 |
| 7:DC:228:ILE:H | 7:DD:226:GLY:H | 1.60 | 0.49 |
| 7:DD:66:VAL:O | 7:DD:84:ARG:NH2 | 2.45 | 0.49 |
| 8:DF:143:ASP:OD1 | 8:DF:144:TRP:N | 2.45 | 0.49 |
| 8:DF:137:VAL:HA | 8:DF:155:VAL:HG12 | 1.93 | 0.49 |
| 11:DI:147:GLU:N | 11:DI:147:GLU:OE1 | 2.45 | 0.49 |
| 12:DJ:126:TYR:HA | 12:GC:230:TYR:HD2 | 1.76 | 0.49 |
| 12:DJ:156:ASP:OD1 | 12:DJ:157:PRO:HD2 | 2.12 | 0.49 |
| 1:EA:344:ASP:O | 1:EA:347:THR:N | 2.44 | 0.49 |
| 1:EB:86:ARG:HG3 | 1:EB:322:ILE:HG22 | 1.93 | 0.49 |
| 2:EC:1014:ASP:CG | 2:EC:1015:ASN:H | 2.15 | 0.49 |
| 2:EC:149:GLU:O | 2:EC:150:SER:OG | 2.18 | 0.49 |
| 1:EB:55:VAL:HG21 | 2:EC:657:TYR:CE1 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:206:PHE:CG | 5:FA:223:VAL:HA | 2.47 | 0.49 |
| 5:FA:316:ILE:HD13 | 6:FC:7:LYS:HG3 | 1.94 | 0.49 |
| 5:FA:490:TRP:CD1 | 5:FA:516:ALA:HA | 2.46 | 0.49 |
| 6:FC:10:VAL:HG22 | 6:FD:13:ARG:HB2 | 1.94 | 0.49 |
| 7:FE:173:ILE:HD11 | 7:FG:174:ALA:HB2 | 1.94 | 0.49 |
| 7:FE:336:GLU:O | 7:FE:340:THR:N | 2.36 | 0.49 |
| 7:FF:221:THR:HG23 | 7:FF:224:TYR:H | 1.77 | 0.49 |
| 7:FE:76:VAL:HG11 | 7:FG:81:LEU:HD22 | 1.94 | 0.49 |
| 8:FH:143:ASP:OD1 | 8:FH:144:TRP:N | 2.45 | 0.49 |
| 4:G:30:LYS:O | 4:G:34:ASP:N | 2.45 | 0.49 |
| 12:GC:30:PRO:HG2 | 12:GC:177:TRP:NE1 | 2.27 | 0.49 |
| 1:GD:278:ALA:HA | 1:GD:316:GLY:HA3 | 1.94 | 0.49 |
| 1:GD:512:SER:OG | 1:GD:513:ASN:N | 2.44 | 0.49 |
| 2:GF:916:TYR:HB3 | 2:GF:1004:PHE:HB3 | 1.94 | 0.49 |
| 2:GF:1013:LYS:HB3 | 3:GG:206:GLU:OE2 | 2.12 | 0.49 |
| 2:GF:193:MET:O | 2:GF:200:TYR:N | 2.36 | 0.49 |
| 2:GF:629:GLU:OE1 | 2:GF:629:GLU:N | 2.40 | 0.49 |
| 4:GI:166:SER:OG | 4:HA:173:SER:N | 2.37 | 0.49 |
| 5:HB:186:TYR:OH | 5:HB:190:ASN:O | 2.19 | 0.49 |
| 5:HB:506:LEU:HB3 | 5:HB:510:GLY:HA2 | 1.93 | 0.49 |
| 5:HB:76:ARG:NH2 | 5:HB:78:THR:OG1 | 2.45 | 0.49 |
| 5:HC:158:ASP:OD1 | 5:HC:159:ILE:N | 2.44 | 0.49 |
| 5:HD:87:ASN:HA | 5:HD:89:TYR:CE2 | 2.47 | 0.49 |
| 12:IF:159:VAL:HG22 | 12:IF:242:THR:HG22 | 1.93 | 0.49 |
| 5:J:102:TRP:HB2 | 5:J:129:ARG:O | 2.13 | 0.49 |
| 5:J:335:ASP:N | 5:J:335:ASP:OD1 | 2.45 | 0.49 |
| 5:J:261:ARG:HB2 | 5:J:383:ILE:HB | 1.93 | 0.49 |
| 5:I:241:THR:HG21 | 5:K:200:LEU:CD1 | 2.42 | 0.49 |
| 5:K:323:THR:CG2 | 5:K:354:THR:HG23 | 2.43 | 0.49 |
| 7:Q:367:VAL:O | 7:Q:389:ASN:HA | 2.12 | 0.49 |
| 12:W:30:PRO:HG2 | 12:W:177:TRP:NE1 | 2.27 | 0.49 |
| 1:X:555:ILE:HG13 | 1:X:556:GLY:N | 2.27 | 0.49 |
| 1:X:636:ASP:N | 1:X:636:ASP:OD1 | 2.44 | 0.49 |
| 1:Y:98:TYR:CE2 | 1:Y:100:PRO:HA | 2.47 | 0.49 |
| 13:YA:13[A]:GLY:O | 13:YA:82[A]:VAL:N | 2.45 | 0.49 |
| 13:YA:266[A]:TRP:O | 13:YA:274[A]:GLN:NE2 | 2.45 | 0.49 |
| 13:YA:490[A]:VAL:O | 13:YC:498[A]:VAL:HA | 2.11 | 0.49 |
| 13:YA:522[E]:VAL:HG11 | 13:YA:526[E]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:557[D]:MET:HG2 | 13:YC:565[D]:TYR:CZ | 2.47 | 0.49 |
| 13:YB:292[F]:PHE:CD1 | 13:YC:364[F]:ALA:HB2 | 2.47 | 0.49 |
| 13:YB:442[A]:THR:HG21 | 13:YC:438[A]:LEU:CD2 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:69[F]:ILE:HG12 | 13:YC:396[F]:GLU:HA | 1.94 | 0.49 |
| 13:YB:13[A]:GLY:O | 13:YB:82[A]:VAL:N | 2.45 | 0.49 |
| 13:YC:81[E]:ARG:HB3 | 13:YC:100[E]:TYR:CZ | 2.47 | 0.49 |
| 13:YB:292[D]:PHE:CD1 | 13:YC:364[D]:ALA:HB2 | 2.47 | 0.49 |
| 13:YC:522[A]:VAL:HG11 | 13:YC:526[A]:GLN:NE2 | 2.28 | 0.49 |
| 13:YC:522[C]:VAL:HG11 | 13:YC:526[C]:GLN:NE2 | 2.27 | 0.49 |
| 13:YB:571[A]:ARG:HB3 | 13:YC:564[A]:GLN:NE2 | 2.27 | 0.49 |
| 14:YD:16[D]:LEU:HB2 | 14:YD:70[D]:ILE:HD13 | 1.94 | 0.49 |
| 13:YB:24[A]:LEU:HD23 | 14:YE:259[A]:LEU:HD22 | 1.92 | 0.49 |
| 14:YE:293[E]:GLU:N | 14:YE:293[E]:GLU:OE1 | 2.45 | 0.49 |
| 14:YE:296[C]:ILE:HD11 | 14:YE:367[C]:ILE:HA | 1.93 | 0.49 |
| 14:YE:296[D]:ILE:HD11 | 14:YE:367[D]:ILE:HA | 1.93 | 0.49 |
| 14:YE:296[B]:ILE:HD11 | 14:YE:367[B]:ILE:HA | 1.93 | 0.49 |
| 14:YF:296[A]:ILE:HD11 | 14:YF:367[A]:ILE:HA | 1.93 | 0.49 |
| 14:YF:47[B]:ARG:O | 14:YF:48[B]:ASN:ND2 | 2.45 | 0.49 |
| 14:YF:72[A]:ILE:O | 14:YF:86[A]:ARG:N | 2.46 | 0.49 |
| 2:Z:173:TYR:CE1 | 2:Z:579:LYS:HE2 | 2.47 | 0.49 |
| 2:Z:371:ILE:HG13 | 2:Z:372:CYS:H | 1.76 | 0.49 |
| 2:Z:58:ASN:OD1 | 2:Z:59:LEU:N | 2.44 | 0.49 |
| 2:Z:821:ILE:HG22 | 2:Z:822:ALA:N | 2.25 | 0.49 |
| 4:AB:139:VAL:HG21 | 4:AB:146:VAL:HG21 | 1.93 | 0.49 |
| 6:AG:70:ILE:HD11 | 6:AH:74:LYS:HG3 | 1.94 | 0.49 |
| 6:AH:35:VAL:HG13 | 6:AH:58:ASP:HB2 | 1.93 | 0.49 |
| 7:AI:417:ASN:HB3 | 7:AI:421:GLY:HA2 | 1.94 | 0.49 |
| 7:AJ:167:GLN:O | 7:AJ:170:ILE:N | 2.45 | 0.49 |
| 1:B:197:VAL:HG22 | 1:B:272:TYR:HB3 | 1.94 | 0.49 |
| 1:B:114:CYS:SG | 1:B:295:ILE:HG23 | 2.53 | 0.49 |
| 1:B:427:ASN:HA | 2:GF:713:ILE:HD12 | 1.93 | 0.49 |
| 1:B:86:ARG:HG3 | 1:B:322:ILE:HG22 | 1.93 | 0.49 |
| 7:BA:196:VAL:HA | 7:BA:199:VAL:HG22 | 1.95 | 0.49 |
| 7:AI:407:SER:N | 7:BA:394:ASP:OD2 | 2.38 | 0.49 |
| 7:BA:405:ARG:NH2 | 7:BA:409:LEU:O | 2.46 | 0.49 |
| 1:BH:116:ASP:HB2 | 1:BH:161:TYR:OH | 2.12 | 0.49 |
| 1:BI:518:ASN:OD1 | 1:BI:535:LEU:HB3 | 2.13 | 0.49 |
| 1:BI:627:PRO:HG3 | 1:BI:632:ILE:HD11 | 1.94 | 0.49 |
| 2:C:1012:LEU:HB2 | 2:C:1027:GLN:OE1 | 2.12 | 0.49 |
| 2:C:433:ASN:HD21 | 2:C:513:PHE:HA | 1.75 | 0.49 |
| 3:CA:225:TYR:CE2 | 3:CA:231:TRP:HB3 | 2.47 | 0.49 |
| 3:CB:72:TRP:NE1 | 3:CB:304:ARG:HD3 | 2.27 | 0.49 |
| 5:CF:249:ASP:OD1 | 5:CG:160:SER:HB2 | 2.11 | 0.49 |
| 5:CF:454:TYR:CD1 | 5:CF:458:THR:HG21 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:506:LEU:HB3 | 5:CF:510:GLY:HA2 | 1.93 | 0.49 |
| 5:CG:115:ASP:HB3 | 5:CG:141:GLY:O | 2.12 | 0.49 |
| 5:CG:147:LYS:HE2 | 5:CG:155:THR:HB | 1.94 | 0.49 |
| 5:CG:159:ILE:HG23 | 5:CG:246:THR:HG21 | 1.94 | 0.49 |
| 5:CH:196:ARG:HD2 | 7:DC:5:THR:OG1 | 2.11 | 0.49 |
| 5:CH:206:PHE:CG | 5:CH:223:VAL:HA | 2.47 | 0.49 |
| 5:CH:87:ASN:HA | 5:CH:89:TYR:CE2 | 2.47 | 0.49 |
| 3:D:7:ILE:HD11 | 3:E:316:PRO:HG2 | 1.93 | 0.49 |
| 7:DB:29:ILE:O | 7:DB:30:THR:OG1 | 2.23 | 0.49 |
| 7:DC:394:ASP:OD2 | 7:DD:407:SER:N | 2.31 | 0.49 |
| 7:DD:123:VAL:O | 7:DD:127:ASN:N | 2.26 | 0.49 |
| 7:DC:295:ILE:HG12 | 7:DD:301:ARG:HD3 | 1.93 | 0.49 |
| 7:DB:339:ARG:NH1 | 7:DD:356:SER:HB2 | 2.27 | 0.49 |
| 10:DH:208:THR:HA | 10:DH:345:GLU:HG2 | 1.94 | 0.49 |
| 1:EA:510:MET:HE1 | 1:EA:623:LEU:HD21 | 1.93 | 0.49 |
| 1:EA:460:ALA:HA | 1:EA:631:VAL:HG12 | 1.93 | 0.49 |
| 1:EB:378:PRO:HG3 | 1:EB:384:LEU:HA | 1.93 | 0.49 |
| 1:EB:518:ASN:OD1 | 1:EB:535:LEU:HB3 | 2.13 | 0.49 |
| 3:ED:63:ASP:HB2 | 3:EE:13:THR:HG23 | 1.93 | 0.49 |
| 4:EH:111:ASN:HD21 | 4:EH:115:SER:N | 2.10 | 0.49 |
| 5:EJ:168:LEU:HA | 5:EJ:241:THR:HG22 | 1.94 | 0.49 |
| 4:F:30:LYS:O | 4:F:34:ASP:N | 2.45 | 0.49 |
| 5:EJ:200:LEU:HD11 | 5:FA:241:THR:HG21 | 1.94 | 0.49 |
| 5:FA:558:ASP:N | 5:FA:558:ASP:OD1 | 2.45 | 0.49 |
| 6:FC:149:HIS:HB3 | 6:FC:152:ASP:O | 2.11 | 0.49 |
| 6:FD:29:VAL:O | 6:FD:32:ARG:N | 2.36 | 0.49 |
| 7:FE:145:SER:O | 7:FE:164:LYS:HE2 | 2.11 | 0.49 |
| 7:FE:417:ASN:HB3 | 7:FE:421:GLY:HA2 | 1.94 | 0.49 |
| 7:FE:451:PHE:CD1 | 7:FE:469:VAL:HG13 | 2.48 | 0.49 |
| 7:FE:471:THR:HA | 7:FG:474:GLY:O | 2.11 | 0.49 |
| 7:FE:339:ARG:NH1 | 7:FG:356:SER:HB2 | 2.27 | 0.49 |
| 7:FF:429:CYS:SG | 7:FG:515:TRP:NE1 | 2.86 | 0.49 |
| 11:GB:138:ASP:HB3 | 11:GB:140:ALA:H | 1.76 | 0.49 |
| 1:GD:543:THR:OG1 | 1:GD:544:ASP:N | 2.45 | 0.49 |
| 1:GD:559:ALA:HB3 | 1:GD:562:ASP:OD2 | 2.11 | 0.49 |
| 2:GF:336:ILE:O | 2:GF:348:ARG:HB2 | 2.12 | 0.49 |
| 2:GF:324:ASP:HB3 | 2:GF:362:LYS:HG2 | 1.95 | 0.49 |
| 2:GF:444:SER:HB2 | 2:GF:512:PRO:HG3 | 1.94 | 0.49 |
| 2:GF:726:PHE:O | 2:GF:729:SER:OG | 2.16 | 0.49 |
| 2:GF:817:LEU:HD11 | 3:GH:252:TYR:CE2 | 2.47 | 0.49 |
| 4:HA:193:HIS:HA | 4:HA:260:TYR:HD1 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:359:GLU:H | 5:HB:370:HIS:C | 2.15 | 0.49 |
| 5:HC:316:ILE:HD13 | 6:HE:7:LYS:HE3 | 1.93 | 0.49 |
| 5:HD:285:LEU:HD21 | 5:HD:375:PHE:H | 1.76 | 0.49 |
| 5:HB:318:GLN:NE2 | 6:HG:4:LEU:HA | 2.27 | 0.49 |
| 7:O:412:PRO:CG | 7:HH:87:TYR:HA | 2.42 | 0.49 |
| 7:HH:159:ALA:HB1 | 7:HI:159:ALA:HB2 | 1.93 | 0.49 |
| 7:HI:382:ARG:HG3 | 7:HI:383:TYR:CD2 | 2.47 | 0.49 |
| 7:HJ:361:PHE:HA | 7:HJ:522:ILE:HA | 1.93 | 0.49 |
| 8:IB:143:ASP:OD1 | 8:IB:144:TRP:N | 2.45 | 0.49 |
| 10:ID:132:SER:HA | 10:ID:209:TRP:NE1 | 2.25 | 0.49 |
| 10:ID:313:PRO:HG2 | 10:ID:351:ILE:HG22 | 1.93 | 0.49 |
| 10:ID:332:LEU:HD21 | 10:ID:340:SER:CB | 2.41 | 0.49 |
| 11:IE:138:ASP:HB3 | 11:IE:140:ALA:H | 1.77 | 0.49 |
| 6:N:29:VAL:O | 6:N:32:ARG:N | 2.36 | 0.49 |
| 7:O:235:GLU:OE1 | 7:O:243:VAL:HG11 | 2.12 | 0.49 |
| 7:O:477:TRP:CZ3 | 7:P:469:VAL:HB | 2.47 | 0.49 |
| 10:U:330:ASN:HB2 | 12:W:189:ARG:NH2 | 2.27 | 0.49 |
| 1:Y:185:ILE:O | 1:Y:235:GLU:HG2 | 2.12 | 0.49 |
| 1:Y:86:ARG:HG3 | 1:Y:322:ILE:HG22 | 1.93 | 0.49 |
| 13:YA:109[C]:ASN:HB3 | 13:YA:112[C]:GLU:HB2 | 1.95 | 0.49 |
| 13:YA:12[A]:VAL:HG21 | 14:YF:256[A]:HIS:CE1 | 2.47 | 0.49 |
| 13:YA:179[A]:MET:SD | 13:YA:279[A]:ASN:ND2 | 2.76 | 0.49 |
| 13:YA:266[D]:TRP:O | 13:YA:274[D]:GLN:NE2 | 2.45 | 0.49 |
| 13:YA:34[A]:LEU:HD13 | 14:YD:163[A]:THR:HG21 | 1.94 | 0.49 |
| 13:YA:416[A]:HIS:CE1 | 13:YA:417[A]:PRO:HD2 | 2.47 | 0.49 |
| 13:YA:67[D]:SER:HB3 | 13:YB:123[D]:ARG:HB2 | 1.94 | 0.49 |
| 13:YB:81[E]:ARG:HB3 | 13:YB:100[E]:TYR:CZ | 2.47 | 0.49 |
| 13:YB:344[F]:LYS:HE2 | 13:YB:344[F]:LYS:HA | 1.93 | 0.49 |
| 13:YB:442[F]:THR:HG21 | 13:YC:438[F]:LEU:CD2 | 2.42 | 0.49 |
| 13:YB:485[D]:ASP:O | 13:YC:478[D]:ASN:N | 2.45 | 0.49 |
| 13:YB:538[F]:VAL:HA | 13:YC:530[F]:VAL:O | 2.12 | 0.49 |
| 13:YB:61[F]:ILE:HG22 | 13:YC:76[F]:PRO:HA | 1.94 | 0.49 |
| 13:YC:344[F]:LYS:HE2 | 13:YC:344[F]:LYS:HA | 1.94 | 0.49 |
| 13:YB:292[C]:PHE:CD1 | 13:YC:364[C]:ALA:HB2 | 2.47 | 0.49 |
| 13:YC:379[A]:PRO:HG2 | 13:YC:429[A]:ARG:CZ | 2.41 | 0.49 |
| 13:YC:416[B]:HIS:CE1 | 13:YC:417[B]:PRO:HD2 | 2.47 | 0.49 |
| 13:YA:430[F]:ARG:HB3 | 13:YC:434[F]:THR:HG21 | 1.93 | 0.49 |
| 14:YD:45[C]:TYR:O | 14:YD:174[C]:ARG:NH2 | 2.46 | 0.49 |
| 14:YD:278[D]:SER:O | 14:YD:279[D]:ARG:NH1 | 2.44 | 0.49 |
| 14:YD:332[D]:GLN:HB3 | 14:YE:61[D]:HIS:NE2 | 2.27 | 0.49 |
| 14:YE:16[C]:LEU:HB2 | 14:YE:70[C]:ILE:HD13 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:332[B]:GLN:OE1 | 14:YF:101[B]:GLY:HA2 | 2.12 | 0.49 |
| 14:YE:373[B]:LYS:HG2 | 14:YE:374[B]:ASN:N | 2.26 | 0.49 |
| 14:YF:16[C]:LEU:HB2 | 14:YF:70[C]:ILE:HD13 | 1.94 | 0.49 |
| 14:YF:45[C]:TYR:O | 14:YF:174[C]:ARG:NH2 | 2.46 | 0.49 |
| 14:YF:293[F]:GLU:N | 14:YF:293[F]:GLU:OE1 | 2.45 | 0.49 |
| 14:YF:293[B]:GLU:OE1 | 14:YF:293[B]:GLU:N | 2.45 | 0.49 |
| 14:YF:296[F]:ILE:HD11 | 14:YF:367[F]:ILE:HA | 1.93 | 0.49 |
| 14:YF:296[D]:ILE:HD11 | 14:YF:367[D]:ILE:HA | 1.93 | 0.49 |
| 2:Z:225:PHE:CE1 | 2:Z:294:PHE:HD2 | 2.29 | 0.49 |
| 2:Z:336:ILE:O | 2:Z:348:ARG:HB2 | 2.12 | 0.49 |
| 2:Z:234:SER:OG | 2:Z:366:TYR:O | 2.25 | 0.49 |
| 1:A:287:SER:HB2 | 14:YF:373[C]:LYS:HD2 | 1.94 | 0.49 |
| 1:A:361:GLN:OE1 | 1:A:362:THR:N | 2.42 | 0.49 |
| 1:A:555:ILE:HG13 | 1:A:556:GLY:N | 2.27 | 0.49 |
| 5:AC:249:ASP:OD1 | 5:AD:160:SER:HB2 | 2.12 | 0.49 |
| 5:AC:569:TYR:CE2 | 5:AE:542:LEU:HD11 | 2.47 | 0.49 |
| 5:AD:312:ARG:HD3 | 5:AD:317:LEU:HD12 | 1.93 | 0.49 |
| 5:AC:407:TYR:CD2 | 5:AD:407:TYR:CD2 | 3.00 | 0.49 |
| 5:AD:491:ASN:ND2 | 5:AD:496:ASP:HB2 | 2.27 | 0.49 |
| 5:AD:590:GLN:OE1 | 5:AE:589:ILE:HA | 2.12 | 0.49 |
| 6:AF:149:HIS:HB3 | 6:AF:152:ASP:O | 2.11 | 0.49 |
| 1:B:98:TYR:CE2 | 1:B:100:PRO:HA | 2.47 | 0.49 |
| 7:AI:260:ARG:HA | 7:BA:263:VAL:O | 2.12 | 0.49 |
| 7:BA:386:ASN:HB2 | 7:BA:387:PRO:HD2 | 1.94 | 0.49 |
| 1:BI:153:ALA:HB2 | 1:BI:163:PRO:HB3 | 1.93 | 0.49 |
| 1:BI:185:ILE:O | 1:BI:235:GLU:HG2 | 2.12 | 0.49 |
| 1:BI:510:MET:SD | 1:BI:602:ILE:HD13 | 2.52 | 0.49 |
| 2:BJ:193:MET:N | 2:BJ:200:TYR:O | 2.37 | 0.49 |
| 2:BJ:314:THR:CG2 | 2:BJ:317:TYR:HB2 | 2.43 | 0.49 |
| 2:BJ:341:LEU:O | 2:BJ:342:SER:HB2 | 2.13 | 0.49 |
| 2:BJ:366:TYR:HB2 | 2:BJ:380:ILE:CD1 | 2.41 | 0.49 |
| 2:BJ:926:PRO:HG2 | 2:BJ:985:GLU:HG2 | 1.94 | 0.49 |
| 2:C:444:SER:HB2 | 2:C:512:PRO:HG3 | 1.94 | 0.49 |
| 2:C:6:PRO:O | 2:C:7:SER:OG | 2.27 | 0.49 |
| 2:C:713:ILE:HD12 | 1:Y:427:ASN:HA | 1.94 | 0.49 |
| 3:CB:3:ASP:OD1 | 3:CB:4:SER:N | 2.45 | 0.49 |
| 4:CD:111:ASN:HD21 | 4:CD:115:SER:N | 2.10 | 0.49 |
| 4:CE:111:ASN:HD21 | 4:CE:115:SER:N | 2.10 | 0.49 |
| 5:CF:262:GLN:HG2 | 5:CF:382:ASN:HD22 | 1.76 | 0.49 |
| 5:CG:264:ARG:HG3 | 5:CG:379:ASP:O | 2.12 | 0.49 |
| 5:CH:206:PHE:HZ | 5:CH:221:GLU:HG2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:CJ:54:SER:HA | 6:DA:164:GLN:HE22 | 1.78 | 0.49 |
| 3:D:117:ALA:O | 3:D:121:ALA:N | 2.45 | 0.49 |
| 3:D:131:TYR:CD2 | 3:D:170:PRO:HG2 | 2.47 | 0.49 |
| 3:D:50:ASN:HB2 | 3:D:56:PHE:CE1 | 2.47 | 0.49 |
| 5:CF:318:GLN:NE2 | 6:DA:4:LEU:HA | 2.27 | 0.49 |
| 7:DC:445:HIS:CE1 | 7:DD:445:HIS:NE2 | 2.81 | 0.49 |
| 7:DC:84:ARG:HH12 | 7:DC:88:PRO:HB3 | 1.76 | 0.49 |
| 7:DC:117:THR:CB | 7:DD:112:ASN:HA | 2.42 | 0.49 |
| 7:DD:171:LYS:O | 7:DD:175:GLN:HG3 | 2.13 | 0.49 |
| 7:DC:36:ILE:HG13 | 7:DD:18:PHE:CE1 | 2.47 | 0.49 |
| 7:DD:211:SER:N | 7:DD:214:THR:OG1 | 2.39 | 0.49 |
| 9:DG:105:ILE:HA | 9:DG:125:GLN:HA | 1.93 | 0.49 |
| 1:EA:229:THR:OG1 | 1:EA:233:ASN:OD1 | 2.30 | 0.49 |
| 1:EA:278:ALA:HA | 1:EA:316:GLY:HA3 | 1.94 | 0.49 |
| 1:EA:282:GLY:N | 1:EA:312:GLY:O | 2.39 | 0.49 |
| 1:EB:189:ASP:HA | 11:GB:121:TYR:CE2 | 2.47 | 0.49 |
| 1:EB:114:CYS:SG | 1:EB:295:ILE:HG23 | 2.53 | 0.49 |
| 1:EB:392:ILE:HG23 | 1:EB:408:ILE:HD13 | 1.94 | 0.49 |
| 2:EC:238:TYR:HB3 | 2:EC:247:VAL:HG12 | 1.94 | 0.49 |
| 3:EE:72:TRP:NE1 | 3:EE:304:ARG:HD3 | 2.27 | 0.49 |
| 5:EI:446:VAL:HG21 | 5:EJ:443:PHE:CD2 | 2.47 | 0.49 |
| 5:EJ:249:ASP:CA | 5:FA:158:ASP:HB3 | 2.42 | 0.49 |
| 8:FH:43:ALA:HB2 | 8:IA:139:GLU:H | 1.77 | 0.49 |
| 1:GD:430:GLN:CD | 1:GD:430:GLN:H | 2.14 | 0.49 |
| 1:GE:114:CYS:SG | 1:GE:295:ILE:HG23 | 2.52 | 0.49 |
| 2:GF:9:THR:HG21 | 3:GH:57:ALA:HB3 | 1.94 | 0.49 |
| 4:GJ:70:HIS:HB2 | 4:GJ:75:TYR:CE2 | 2.47 | 0.49 |
| 4:H:70:HIS:HB2 | 4:H:75:TYR:CE2 | 2.47 | 0.49 |
| 4:H:79:VAL:N | 4:H:97:ILE:O | 2.31 | 0.49 |
| 5:HC:115:ASP:HB3 | 5:HC:141:GLY:O | 2.12 | 0.49 |
| 5:HC:290:SER:N | 5:HC:371:PHE:O | 2.45 | 0.49 |
| 5:HC:312:ARG:HD3 | 5:HC:317:LEU:HD12 | 1.93 | 0.49 |
| 5:HD:138:CYS:SG | 5:HD:140:PRO:HD2 | 2.52 | 0.49 |
| 5:HD:200:LEU:HD23 | 5:HD:210:SER:HA | 1.93 | 0.49 |
| 5:HD:323:THR:CG2 | 5:HD:354:THR:HG23 | 2.43 | 0.49 |
| 6:HF:122:ALA:O | 6:HF:126:VAL:HG23 | 2.12 | 0.49 |
| 7:HH:509:GLY:HA3 | 7:HI:441:GLN:NE2 | 2.28 | 0.49 |
| 7:HI:515:TRP:CD1 | 7:HJ:440:GLN:HB3 | 2.48 | 0.49 |
| 7:HJ:66:VAL:O | 7:HJ:84:ARG:NH2 | 2.45 | 0.49 |
| 5:J:258:TYR:O | 5:J:259:THR:OG1 | 2.24 | 0.49 |
| 5:J:590:GLN:OE1 | 5:K:589:ILE:HA | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:N:35:VAL:HG13 | 6:N:58:ASP:HB2 | 1.93 | 0.49 |
| 7:O:211:SER:O | 7:O:215:PHE:N | 2.43 | 0.49 |
| 7:O:289:GLN:HB2 | 7:P:286:ASP:O | 2.12 | 0.49 |
| 7:Q:66:VAL:O | 7:Q:84:ARG:NH2 | 2.45 | 0.49 |
| 1:B:52:ARG:HE | 9:T:13:PRO:HB3 | 1.77 | 0.49 |
| 1:X:229:THR:OG1 | 1:X:233:ASN:OD1 | 2.30 | 0.49 |
| 1:X:566:ASN:HB3 | 1:X:569:ILE:HG13 | 1.94 | 0.49 |
| 1:Y:197:VAL:HG22 | 1:Y:272:TYR:HB3 | 1.94 | 0.49 |
| 1:Y:461:LYS:HE3 | 1:Y:630:ASP:OD1 | 2.12 | 0.49 |
| 13:YA:109[E]:ASN:HB3 | 13:YA:112[E]:GLU:HB2 | 1.93 | 0.49 |
| 13:YA:270[A]:ASN:O | 13:YA:274[A]:GLN:N | 2.42 | 0.49 |
| 13:YA:266[B]:TRP:O | 13:YA:274[B]:GLN:NE2 | 2.46 | 0.49 |
| 13:YA:344[B]:LYS:HE2 | 13:YA:344[B]:LYS:HA | 1.94 | 0.49 |
| 13:YA:416[F]:HIS:CE1 | 13:YA:417[F]:PRO:HD2 | 2.47 | 0.49 |
| 13:YA:428[A]:GLY:HA3 | 13:YC:418[A]:THR:HG21 | 1.93 | 0.49 |
| 13:YA:430[D]:ARG:HB3 | 13:YC:434[D]:THR:HG21 | 1.93 | 0.49 |
| 13:YA:95[B]:ILE:HD11 | 13:YB:83[B]:TYR:CZ | 2.47 | 0.49 |
| 13:YB:344[E]:LYS:HE2 | 13:YB:344[E]:LYS:HA | 1.94 | 0.49 |
| 13:YA:474[A]:ILE:HG12 | 13:YB:466[A]:ASN:HB2 | 1.93 | 0.49 |
| 13:YA:474[C]:ILE:HG12 | 13:YB:466[C]:ASN:HB2 | 1.93 | 0.49 |
| 13:YB:490[B]:VAL:HG11 | 13:YC:486[B]:GLU:CB | 2.43 | 0.49 |
| 13:YB:538[D]:VAL:HA | 13:YC:530[D]:VAL:O | 2.12 | 0.49 |
| 13:YB:61[B]:ILE:HG12 | 13:YC:60[B]:PRO:CD | 2.42 | 0.49 |
| 13:YC:344[C]:LYS:HA | 13:YC:344[C]:LYS:HE2 | 1.94 | 0.49 |
| 13:YC:436[E]:ASP:OD2 | 13:YC:437[E]:ASN:N | 2.45 | 0.49 |
| 13:YC:13[A]:GLY:O | 13:YC:82[A]:VAL:N | 2.45 | 0.49 |
| 14:YD:45[F]:TYR:O | 14:YD:174[F]:ARG:NH2 | 2.45 | 0.49 |
| 14:YD:296[B]:ILE:HD11 | 14:YD:367[B]:ILE:HA | 1.93 | 0.49 |
| 14:YD:296[E]:ILE:HD11 | 14:YD:367[E]:ILE:HA | 1.93 | 0.49 |
| 14:YD:296[F]:ILE:HD11 | 14:YD:367[F]:ILE:HA | 1.93 | 0.49 |
| 14:YD:373[A]:LYS:HG2 | 14:YD:374[A]:ASN:N | 2.27 | 0.49 |
| 14:YE:45[C]:TYR:O | 14:YE:174[C]:ARG:NH2 | 2.46 | 0.49 |
| 13:YC:34[B]:LEU:HD13 | 14:YF:163[B]:THR:HG21 | 1.94 | 0.49 |
| 14:YF:293[A]:GLU:N | 14:YF:293[A]:GLU:OE1 | 2.45 | 0.49 |
| 14:YF:296[E]:ILE:HD11 | 14:YF:367[E]:ILE:HA | 1.94 | 0.49 |
| 14:YF:296[B]:ILE:HD11 | 14:YF:367[B]:ILE:HA | 1.93 | 0.49 |
| 14:YF:373[A]:LYS:HG2 | 14:YF:374[A]:ASN:N | 2.28 | 0.49 |
| 14:YF:47[A]:ARG:O | 14:YF:48[A]:ASN:ND2 | 2.45 | 0.49 |
| 2:Z:18:ALA:HA | 2:Z:102:THR:HB | 1.94 | 0.49 |
| 2:Z:341:LEU:O | 2:Z:342:SER:HB2 | 2.13 | 0.49 |
| 2:Z:796:THR:HG22 | 2:Z:812:THR:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:ZA:2[F]:SER:HB3 | 15:ZA:77[F]:MET:HB3 | 1.93 | 0.49 |
| 4:AA:111:ASN:HD21 | 4:AA:115:SER:N | 2.10 | 0.49 |
| 4:AA:168:PHE:CE1 | 4:AB:161:ASN:HB3 | 2.47 | 0.49 |
| 5:AC:194:LYS:HE3 | 5:AE:198:ASN:HD22 | 1.76 | 0.49 |
| 5:AC:275:SER:OG | 5:AC:282:VAL:HG12 | 2.13 | 0.49 |
| 5:AD:102:TRP:HB2 | 5:AD:129:ARG:O | 2.12 | 0.49 |
| 5:AE:265:LEU:HG | 5:AE:379:ASP:HB2 | 1.94 | 0.49 |
| 5:AE:490:TRP:CD1 | 5:AE:516:ALA:HA | 2.46 | 0.49 |
| 5:AE:87:ASN:HA | 5:AE:89:TYR:CE2 | 2.47 | 0.49 |
| 7:AJ:382:ARG:HG3 | 7:AJ:383:TYR:CD2 | 2.47 | 0.49 |
| 1:B:510:MET:SD | 1:B:602:ILE:HD13 | 2.52 | 0.49 |
| 7:AJ:117:THR:CB | 7:BA:112:ASN:HA | 2.43 | 0.49 |
| 2:BJ:1012:LEU:HB2 | 2:BJ:1027:GLN:OE1 | 2.12 | 0.49 |
| 2:BJ:152:GLN:N | 2:BJ:152:GLN:OE1 | 2.31 | 0.49 |
| 2:BJ:324:ASP:HB3 | 2:BJ:362:LYS:HG2 | 1.95 | 0.49 |
| 2:C:319:TYR:CD1 | 2:C:328:TYR:HB2 | 2.47 | 0.49 |
| 2:C:324:ASP:HB3 | 2:C:362:LYS:HG2 | 1.95 | 0.49 |
| 2:C:629:GLU:OE1 | 2:C:629:GLU:N | 2.40 | 0.49 |
| 2:C:682:GLN:O | 2:C:685:ASN:HB3 | 2.12 | 0.49 |
| 2:C:947:VAL:O | 3:D:118:PRO:HD2 | 2.13 | 0.49 |
| 4:CC:4:GLN:NE2 | 4:CE:61:ILE:O | 2.39 | 0.49 |
| 5:CF:20:ARG:HH12 | 5:CF:24:ILE:HD12 | 1.78 | 0.49 |
| 5:CF:96:ARG:HD3 | 5:CF:151:ILE:HD11 | 1.94 | 0.49 |
| 5:CG:206:PHE:CD2 | 5:CG:223:VAL:HA | 2.47 | 0.49 |
| 5:CG:261:ARG:NE | 5:CG:297:GLY:O | 2.30 | 0.49 |
| 5:CG:590:GLN:OE1 | 5:CH:589:ILE:HA | 2.13 | 0.49 |
| 5:CH:275:SER:HA | 5:CH:280:ILE:HG22 | 1.92 | 0.49 |
| 3:D:216:LEU:HD23 | 3:D:236:PHE:HB3 | 1.93 | 0.49 |
| 7:DB:176:ILE:HG23 | 7:DB:177:ALA:N | 2.28 | 0.49 |
| 7:DB:452:GLY:HA3 | 7:DD:480:ARG:O | 2.13 | 0.49 |
| 7:DC:221:THR:HG23 | 7:DC:224:TYR:H | 1.77 | 0.49 |
| 12:DJ:16:PHE:N | 12:GC:166:SER:OG | 2.45 | 0.49 |
| 3:E:72:TRP:HZ3 | 3:E:275:ILE:HD13 | 1.77 | 0.49 |
| 1:EA:52:ARG:HH21 | 9:FJ:25:ARG:HB3 | 1.76 | 0.49 |
| 1:EA:69:GLN:HE21 | 11:GB:25:MET:CE | 2.25 | 0.49 |
| 2:EC:916:TYR:HB3 | 2:EC:1004:PHE:HB3 | 1.93 | 0.49 |
| 2:EC:408:HIS:HB3 | 2:EC:410:GLU:CD | 2.32 | 0.49 |
| 3:ED:232:GLN:N | 3:ED:232:GLN:OE1 | 2.42 | 0.49 |
| 5:EJ:102:TRP:HB2 | 5:EJ:129:ARG:O | 2.12 | 0.49 |
| 5:EJ:159:ILE:HG23 | 5:EJ:246:THR:HG21 | 1.94 | 0.49 |
| 5:EI:407:TYR:HD2 | 5:EJ:407:TYR:CE2 | 2.31 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:139:VAL:HG21 | 4:F:146:VAL:HG21 | 1.94 | 0.49 |
| 4:F:193:HIS:HA | 4:F:260:TYR:HD1 | 1.77 | 0.49 |
| 4:F:70:HIS:HB2 | 4:F:75:TYR:CE2 | 2.47 | 0.49 |
| 5:FA:285:LEU:HD21 | 5:FA:375:PHE:H | 1.76 | 0.49 |
| 6:FB:122:ALA:O | 6:FB:126:VAL:HG23 | 2.12 | 0.49 |
| 6:FC:73:ASN:HD21 | 6:FC:215:PHE:HE2 | 1.59 | 0.49 |
| 6:FD:147:LYS:O | 6:FD:157:GLU:N | 2.44 | 0.49 |
| 7:FE:134:SER:HB3 | 7:FE:140:GLY:N | 2.28 | 0.49 |
| 7:FE:140:GLY:O | 7:FG:141:VAL:HG23 | 2.13 | 0.49 |
| 7:FF:236:VAL:O | 7:FF:253:ARG:NH1 | 2.46 | 0.49 |
| 7:FE:399:PHE:HD2 | 7:FG:514:PRO:HG2 | 1.76 | 0.49 |
| 10:GA:330:ASN:HB2 | 12:GC:189:ARG:NH2 | 2.27 | 0.49 |
| 1:GE:444:ILE:O | 1:GE:447:TYR:N | 2.45 | 0.49 |
| 1:GE:98:TYR:CE2 | 1:GE:100:PRO:HA | 2.47 | 0.49 |
| 2:GF:17:SER:HA | 2:GF:106:ASN:HB3 | 1.93 | 0.49 |
| 3:GG:117:ALA:O | 3:GG:121:ALA:N | 2.45 | 0.49 |
| 3:GH:72:TRP:NE1 | 3:GH:304:ARG:HD3 | 2.27 | 0.49 |
| 4:G:113:ASN:ND2 | 4:H:103:LEU:HD21 | 2.19 | 0.49 |
| 4:H:111:ASN:HD21 | 4:H:115:SER:N | 2.10 | 0.49 |
| 5:HC:289:LYS:HD2 | 5:HC:372:ASP:HB3 | 1.95 | 0.49 |
| 5:HC:416:ILE:O | 5:HC:438:SER:HA | 2.13 | 0.49 |
| 5:HD:558:ASP:OD1 | 5:HD:558:ASP:N | 2.45 | 0.49 |
| 6:HF:149:HIS:HB3 | 6:HF:152:ASP:O | 2.11 | 0.49 |
| 6:HG:4:LEU:HD23 | 6:HG:5:ASN:N | 2.27 | 0.49 |
| 7:HH:451:PHE:CD1 | 7:HH:469:VAL:HG13 | 2.48 | 0.49 |
| 7:HI:146:SER:HA | 7:HI:164:LYS:HZ2 | 1.75 | 0.49 |
| 7:HJ:405:ARG:NH2 | 7:HJ:409:LEU:O | 2.46 | 0.49 |
| 8:FI:117:ALA:HA | 8:IB:77:GLU:OE2 | 2.13 | 0.49 |
| 5:J:2:LYS:H | 5:K:41:ASP:HB3 | 1.78 | 0.49 |
| 5:I:407:TYR:CD2 | 5:J:407:TYR:CD2 | 3.00 | 0.49 |
| 5:K:138:CYS:SG | 5:K:140:PRO:HD2 | 2.52 | 0.49 |
| 5:K:87:ASN:HA | 5:K:89:TYR:CE2 | 2.47 | 0.49 |
| 6:M:147:LYS:O | 6:M:157:GLU:N | 2.44 | 0.49 |
| 7:O:442:MET:HA | 7:Q:512:THR:HA | 1.94 | 0.49 |
| 7:O:191:VAL:C | 7:P:188:GLN:HA | 2.33 | 0.49 |
| 7:Q:361:PHE:HA | 7:Q:522:ILE:HA | 1.93 | 0.49 |
| 5:J:196:ARG:NE | 7:Q:5:THR:HG23 | 2.27 | 0.49 |
| 8:R:79:HIS:HE2 | 8:IA:115:GLN:HG2 | 1.78 | 0.49 |
| 1:X:63:ASN:O | 1:X:66:TYR:N | 2.46 | 0.49 |
| 1:X:64:THR:HA | 1:X:67:ILE:HG22 | 1.94 | 0.49 |
| 13:YA:109[A]:ASN:HB3 | 13:YA:112[A]:GLU:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:123[A]:ARG:HB2 | 13:YC:67[A]:SER:HB3 | 1.94 | 0.49 |
| 13:YA:367[D]:PRO:HA | 13:YC:315[D]:LEU:HD23 | 1.94 | 0.49 |
| 13:YA:522[A]:VAL:HG11 | 13:YA:526[A]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:522[C]:VAL:HG11 | 13:YA:526[C]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:563[B]:GLY:N | 13:YB:555[B]:ALA:O | 2.45 | 0.49 |
| 13:YA:563[E]:GLY:N | 13:YB:555[E]:ALA:O | 2.45 | 0.49 |
| 13:YA:57[E]:VAL:HG21 | 13:YA:75[E]:GLY:HA2 | 1.95 | 0.49 |
| 13:YB:13[D]:GLY:O | 13:YB:82[D]:VAL:N | 2.45 | 0.49 |
| 13:YB:490[C]:VAL:HG11 | 13:YC:486[C]:GLU:CB | 2.43 | 0.49 |
| 13:YA:563[A]:GLY:N | 13:YB:555[A]:ALA:O | 2.45 | 0.49 |
| 13:YB:76[A]:PRO:C | 13:YB:98[A]:GLY:HA2 | 2.33 | 0.49 |
| 13:YA:430[E]:ARG:HB3 | 13:YC:434[E]:THR:HG21 | 1.93 | 0.49 |
| 13:YC:436[B]:ASP:OD2 | 13:YC:437[B]:ASN:N | 2.45 | 0.49 |
| 13:YB:442[D]:THR:HG21 | 13:YC:438[D]:LEU:CD2 | 2.42 | 0.49 |
| 13:YA:473[F]:GLN:HA | 13:YC:481[F]:PHE:O | 2.12 | 0.49 |
| 13:YC:522[F]:VAL:HG11 | 13:YC:526[F]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:123[D]:ARG:HB2 | 13:YC:67[D]:SER:HB3 | 1.94 | 0.49 |
| 13:YC:76[A]:PRO:C | 13:YC:98[A]:GLY:HA2 | 2.33 | 0.49 |
| 14:YD:293[E]:GLU:OE1 | 14:YD:293[E]:GLU:N | 2.45 | 0.49 |
| 11:V:182:ASN:ND2 | 14:YD:327[A]:ASN:HD22 | 2.10 | 0.49 |
| 14:YE:332[F]:GLN:HB3 | 14:YF:61[F]:HIS:NE2 | 2.28 | 0.49 |
| 14:YE:296[F]:ILE:HD11 | 14:YE:367[F]:ILE:HA | 1.93 | 0.49 |
| 14:YE:373[C]:LYS:HG2 | 14:YE:374[C]:ASN:N | 2.26 | 0.49 |
| 1:EA:130:ARG:HD3 | 14:YF:181[A]:GLY:HA2 | 1.93 | 0.49 |
| 14:YF:47[E]:ARG:O | 14:YF:48[E]:ASN:ND2 | 2.45 | 0.49 |
| 2:Z:238:TYR:HB3 | 2:Z:247:VAL:HG12 | 1.94 | 0.49 |
| 2:Z:682:GLN:O | 2:Z:685:ASN:HB3 | 2.12 | 0.49 |
| 2:Z:934:ALA:HB2 | 2:Z:998:GLY:HA2 | 1.93 | 0.49 |
| 1:A:645:ASP:OD1 | 1:A:645:ASP:N | 2.45 | 0.49 |
| 5:AC:149:LYS:HG2 | 5:AC:150:GLN:N | 2.27 | 0.49 |
| 5:AD:11:VAL:HG13 | 5:AE:20:ARG:HG2 | 1.95 | 0.49 |
| 5:AD:206:PHE:CD2 | 5:AD:223:VAL:HA | 2.47 | 0.49 |
| 5:AD:267:ASP:OD1 | 5:AD:285:LEU:HB2 | 2.12 | 0.49 |
| 5:AC:182:ARG:NH2 | 5:AD:299:ILE:HG21 | 2.28 | 0.49 |
| 5:AD:320:LEU:HG | 5:AD:357:SER:CB | 2.42 | 0.49 |
| 5:AD:392:THR:OG1 | 5:AE:305:ASN:ND2 | 2.45 | 0.49 |
| 5:AD:416:ILE:O | 5:AD:438:SER:HA | 2.13 | 0.49 |
| 5:AE:323:THR:CG2 | 5:AE:354:THR:HG23 | 2.43 | 0.49 |
| 6:AG:147:LYS:O | 6:AG:157:GLU:N | 2.44 | 0.49 |
| 6:AG:4:LEU:HD23 | 6:AG:5:ASN:N | 2.27 | 0.49 |
| 7:AI:76:VAL:HG11 | 7:BA:81:LEU:HD22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:476:ASP:OD2 | 7:AJ:454:HIS:HE1 | 1.95 | 0.49 |
| 7:AJ:54:THR:HG22 | 7:AJ:55:LYS:O | 2.13 | 0.49 |
| 1:B:461:LYS:HE3 | 1:B:630:ASP:OD1 | 2.12 | 0.49 |
| 1:B:649:GLN:OE1 | 1:B:649:GLN:N | 2.32 | 0.49 |
| 8:BB:143:ASP:OD1 | 8:BB:144:TRP:N | 2.45 | 0.49 |
| 9:BD:20:ASN:HA | 1:BI:311:VAL:CG1 | 2.38 | 0.49 |
| 1:BI:19:GLU:HG2 | 1:BI:19:GLU:O | 2.12 | 0.49 |
| 1:BI:86:ARG:HG3 | 1:BI:322:ILE:HG22 | 1.93 | 0.49 |
| 1:BI:392:ILE:HG23 | 1:BI:408:ILE:HD13 | 1.94 | 0.49 |
| 2:BJ:321:VAL:HB | 2:BJ:326:VAL:HG12 | 1.94 | 0.49 |
| 2:BJ:713:ILE:HD12 | 1:EB:427:ASN:HA | 1.95 | 0.49 |
| 2:C:321:VAL:HB | 2:C:326:VAL:HG12 | 1.94 | 0.49 |
| 1:B:227:ARG:NE | 2:C:694:TYR:CZ | 2.80 | 0.49 |
| 5:CF:496:ASP:HB3 | 5:CF:500:ALA:HB2 | 1.95 | 0.49 |
| 5:CG:419:ASP:OD1 | 5:CG:420:VAL:N | 2.45 | 0.49 |
| 7:DB:134:SER:HB3 | 7:DB:140:GLY:N | 2.28 | 0.49 |
| 7:DD:87:TYR:HD1 | 7:DD:88:PRO:O | 1.96 | 0.49 |
| 3:E:193:GLU:HG2 | 3:E:224:GLY:HA3 | 1.95 | 0.49 |
| 3:E:61:PRO:HG3 | 3:E:314:ASN:OD1 | 2.12 | 0.49 |
| 1:EB:209:TRP:CZ3 | 1:EB:212:LYS:NZ | 2.69 | 0.49 |
| 1:EB:117:ALA:HB3 | 1:EB:294:ASN:HA | 1.95 | 0.49 |
| 1:EB:526:PRO:HB2 | 1:EB:528:THR:HG23 | 1.94 | 0.49 |
| 2:EC:228:ARG:HD2 | 5:FA:556:GLN:HE22 | 1.78 | 0.49 |
| 2:EC:324:ASP:HB3 | 2:EC:362:LYS:HG2 | 1.95 | 0.49 |
| 2:EC:644:ASP:O | 11:GB:84:TYR:OH | 2.28 | 0.49 |
| 3:ED:216:LEU:HD23 | 3:ED:236:PHE:HB3 | 1.93 | 0.49 |
| 4:EG:172:GLU:HA | 4:EH:166:SER:H | 1.75 | 0.49 |
| 5:EI:196:ARG:HD3 | 7:FE:5:THR:HG23 | 1.93 | 0.49 |
| 5:EI:391:GLY:O | 5:EI:392:THR:OG1 | 2.23 | 0.49 |
| 5:EI:454:TYR:CD1 | 5:EI:458:THR:HG21 | 2.47 | 0.49 |
| 5:EI:76:ARG:NH2 | 5:EI:78:THR:OG1 | 2.45 | 0.49 |
| 5:EJ:312:ARG:HD3 | 5:EJ:317:LEU:HD12 | 1.93 | 0.49 |
| 5:EJ:289:LYS:HD2 | 5:EJ:372:ASP:HB3 | 1.95 | 0.49 |
| 5:EJ:313:PHE:HE1 | 6:FB:8:ALA:HB1 | 1.77 | 0.49 |
| 7:FE:176:ILE:HG23 | 7:FE:177:ALA:N | 2.28 | 0.49 |
| 7:FE:235:GLU:OE1 | 7:FE:243:VAL:HG11 | 2.12 | 0.49 |
| 7:FE:255:SER:O | 7:FE:278:SER:OG | 2.29 | 0.49 |
| 7:FF:54:THR:HG22 | 7:FF:55:LYS:O | 2.13 | 0.49 |
| 7:FF:84:ARG:HH12 | 7:FF:88:PRO:HB3 | 1.76 | 0.49 |
| 7:FG:361:PHE:HA | 7:FG:522:ILE:HA | 1.93 | 0.49 |
| 7:FG:87:TYR:HD1 | 7:FG:88:PRO:O | 1.96 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FI:137:VAL:HA | 8:FI:155:VAL:HG12 | 1.94 | 0.49 |
| 4:G:70:HIS:HB2 | 4:G:75:TYR:CE2 | 2.47 | 0.49 |
| 1:GD:411:PRO:HG2 | 1:GD:413:TYR:HD2 | 1.77 | 0.49 |
| 2:GF:173:TYR:CE1 | 2:GF:579:LYS:HE2 | 2.47 | 0.49 |
| 5:HB:149:LYS:HG2 | 5:HB:150:GLN:N | 2.27 | 0.49 |
| 5:HB:290:SER:CB | 5:HB:371:PHE:H | 2.26 | 0.49 |
| 5:HC:206:PHE:CD2 | 5:HC:223:VAL:HA | 2.48 | 0.49 |
| 5:HC:264:ARG:HG3 | 5:HC:379:ASP:O | 2.12 | 0.49 |
| 7:HH:97:LEU:HD23 | 7:HJ:97:LEU:HD21 | 1.95 | 0.49 |
| 7:HI:236:VAL:O | 7:HI:253:ARG:NH1 | 2.46 | 0.49 |
| 7:HI:84:ARG:HH12 | 7:HI:88:PRO:HB3 | 1.76 | 0.49 |
| 7:HJ:386:ASN:HB2 | 7:HJ:387:PRO:HD2 | 1.94 | 0.49 |
| 7:HH:452:GLY:HA2 | 7:HJ:482:TYR:CD2 | 2.48 | 0.49 |
| 7:HJ:338:ASP:HB2 | 7:HJ:527:GLU:OE2 | 2.12 | 0.49 |
| 7:HJ:65:GLU:O | 7:HJ:69:GLY:N | 2.46 | 0.49 |
| 8:IB:137:VAL:HA | 8:IB:155:VAL:HG12 | 1.93 | 0.49 |
| 12:IF:158:LEU:HD21 | 12:IF:216:PHE:CE1 | 2.48 | 0.49 |
| 12:IF:30:PRO:HG2 | 12:IF:177:TRP:NE1 | 2.27 | 0.49 |
| 5:K:558:ASP:HB2 | 5:K:559:PRO:HD2 | 1.94 | 0.49 |
| 7:P:78:PRO:HB2 | 7:Q:69:GLY:HA2 | 1.93 | 0.49 |
| 7:Q:118:PRO:O | 7:Q:122:THR:N | 2.41 | 0.49 |
| 7:Q:73:THR:HG23 | 7:Q:74:LYS:H | 1.78 | 0.49 |
| 13:YA:16[A]:GLU:CD | 13:YA:30[A]:ARG:HH11 | 2.16 | 0.49 |
| 13:YA:266[E]:TRP:O | 13:YA:274[E]:GLN:NE2 | 2.46 | 0.49 |
| 13:YA:407[E]:PRO:HB3 | 13:YC:232[E]:ASN:HB3 | 1.93 | 0.49 |
| 13:YA:436[B]:ASP:OD2 | 13:YA:437[B]:ASN:N | 2.45 | 0.49 |
| 13:YA:564[D]:GLN:HE22 | 13:YC:571[D]:ARG:HD3 | 1.77 | 0.49 |
| 13:YB:109[F]:ASN:HB3 | 13:YB:112[F]:GLU:HB2 | 1.95 | 0.49 |
| 13:YB:416[D]:HIS:CE1 | 13:YB:417[D]:PRO:HD2 | 2.47 | 0.49 |
| 13:YB:490[D]:VAL:HG11 | 13:YC:486[D]:GLU:CB | 2.42 | 0.49 |
| 13:YB:522[A]:VAL:HG11 | 13:YB:526[A]:GLN:NE2 | 2.27 | 0.49 |
| 13:YB:522[B]:VAL:HG11 | 13:YB:526[B]:GLN:NE2 | 2.27 | 0.49 |
| 13:YB:522[E]:VAL:HG11 | 13:YB:526[E]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:563[F]:GLY:N | 13:YB:555[F]:ALA:O | 2.45 | 0.49 |
| 13:YB:66[D]:MET:HE2 | 13:YC:122[D]:PRO:HB3 | 1.95 | 0.49 |
| 13:YC:266[F]:TRP:O | 13:YC:274[F]:GLN:NE2 | 2.45 | 0.49 |
| 13:YB:485[A]:ASP:O | 13:YC:478[A]:ASN:N | 2.45 | 0.49 |
| 13:YC:522[E]:VAL:HG11 | 13:YC:526[E]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:24[E]:LEU:HD23 | 14:YD:259[E]:LEU:CD2 | 2.43 | 0.49 |
| 14:YD:301[F]:MET:HA | 14:YD:304[F]:TYR:CD2 | 2.47 | 0.49 |
| 14:YD:332[B]:GLN:HB3 | 14:YE:61[B]:HIS:NE2 | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:47[C]:ARG:O | 14:YD:48[C]:ASN:ND2 | 2.45 | 0.49 |
| 14:YD:54[B]:PHE:CZ | 14:YD:105[B]:ILE:HD11 | 2.48 | 0.49 |
| 14:YD:97[C]:VAL:HG21 | 14:YF:332[C]:GLN:NE2 | 2.28 | 0.49 |
| 14:YE:45[B]:TYR:O | 14:YE:174[B]:ARG:NH2 | 2.45 | 0.49 |
| 14:YE:278[E]:SER:O | 14:YE:279[E]:ARG:NH1 | 2.43 | 0.49 |
| 14:YF:45[B]:TYR:O | 14:YF:174[B]:ARG:NH2 | 2.45 | 0.49 |
| 1:A:130:ARG:HD3 | 14:YF:181[C]:GLY:HA2 | 1.93 | 0.49 |
| 14:YF:373[F]:LYS:HG2 | 14:YF:374[F]:ASN:N | 2.27 | 0.49 |
| 14:YF:45[F]:TYR:O | 14:YF:174[F]:ARG:NH2 | 2.45 | 0.49 |
| 1:A:378:PRO:HG3 | 1:A:384:LEU:HG | 1.95 | 0.49 |
| 1:A:647:ARG:HH11 | 1:A:650:TYR:HE2 | 1.60 | 0.49 |
| 4:AA:194:ARG:HE | 4:AA:259:ASN:HA | 1.78 | 0.49 |
| 5:AD:264:ARG:HG3 | 5:AD:379:ASP:O | 2.12 | 0.49 |
| 5:AD:289:LYS:HD2 | 5:AD:372:ASP:HB3 | 1.95 | 0.49 |
| 5:AD:335:ASP:N | 5:AD:335:ASP:OD1 | 2.45 | 0.49 |
| 5:AD:415:ASP:HB2 | 5:AD:440:GLN:HE22 | 1.76 | 0.49 |
| 6:AH:122:ALA:O | 6:AH:126:VAL:HG23 | 2.12 | 0.49 |
| 7:AI:134:SER:HB3 | 7:AI:140:GLY:N | 2.28 | 0.49 |
| 7:AI:289:GLN:HB2 | 7:AJ:286:ASP:O | 2.13 | 0.49 |
| 1:B:392:ILE:HG23 | 1:B:408:ILE:HD13 | 1.94 | 0.49 |
| 1:B:522:LYS:HD2 | 1:B:530:LEU:HD13 | 1.95 | 0.49 |
| 7:BA:375:TYR:HE2 | 7:BA:390:PRO:HB2 | 1.77 | 0.49 |
| 7:AI:452:GLY:HA2 | 7:BA:482:TYR:CD2 | 2.48 | 0.49 |
| 7:BA:87:TYR:HD1 | 7:BA:88:PRO:O | 1.96 | 0.49 |
| 11:BF:146:TYR:CE2 | 11:BF:150:LEU:HD23 | 2.48 | 0.49 |
| 1:BH:111:MET:SD | 1:BH:304:PRO:HB3 | 2.52 | 0.49 |
| 1:BI:229:THR:OG1 | 1:BI:231:ASP:OD1 | 2.31 | 0.49 |
| 5:CF:149:LYS:HG2 | 5:CF:150:GLN:N | 2.27 | 0.49 |
| 5:CF:194:LYS:O | 5:CF:242:VAL:HA | 2.13 | 0.49 |
| 5:CF:407:TYR:CD2 | 5:CG:407:TYR:CD2 | 3.01 | 0.49 |
| 5:CG:11:VAL:HG13 | 5:CH:20:ARG:HG2 | 1.95 | 0.49 |
| 5:CG:491:ASN:ND2 | 5:CG:496:ASP:HB2 | 2.27 | 0.49 |
| 5:CH:265:LEU:HG | 5:CH:379:ASP:HB2 | 1.94 | 0.49 |
| 5:CG:2:LYS:H | 5:CH:41:ASP:HB3 | 1.77 | 0.49 |
| 6:CI:147:LYS:O | 6:CI:157:GLU:N | 2.44 | 0.49 |
| 5:CF:340:VAL:HG21 | 6:CJ:174:TYR:H | 1.77 | 0.49 |
| 6:CJ:30:MET:O | 6:CJ:32:ARG:HG2 | 2.13 | 0.49 |
| 7:DC:382:ARG:HG3 | 7:DC:383:TYR:CD2 | 2.47 | 0.49 |
| 7:DB:442:MET:HA | 7:DD:512:THR:HA | 1.94 | 0.49 |
| 7:DD:65:GLU:O | 7:DD:69:GLY:N | 2.46 | 0.49 |
| 1:EA:555:ILE:HG13 | 1:EA:556:GLY:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:19:GLU:O | 1:EB:19:GLU:HG2 | 2.13 | 0.49 |
| 1:EB:229:THR:OG1 | 1:EB:231:ASP:OD1 | 2.31 | 0.49 |
| 1:EB:106:ALA:HB2 | 1:EB:280:ALA:HB1 | 1.93 | 0.49 |
| 2:EC:336:ILE:O | 2:EC:348:ARG:HB2 | 2.12 | 0.49 |
| 2:EC:341:LEU:O | 2:EC:342:SER:HB2 | 2.13 | 0.49 |
| 2:EC:1013:LYS:HB3 | 3:ED:206:GLU:OE2 | 2.12 | 0.49 |
| 3:EE:221:THR:O | 3:EE:224:GLY:N | 2.37 | 0.49 |
| 3:EE:64:SER:HG | 3:EE:67:GLY:H | 1.57 | 0.49 |
| 4:EF:30:LYS:O | 4:EF:34:ASP:N | 2.45 | 0.49 |
| 5:EI:96:ARG:HD3 | 5:EI:151:ILE:HD11 | 1.94 | 0.49 |
| 5:EJ:267:ASP:OD1 | 5:EJ:285:LEU:HB2 | 2.12 | 0.49 |
| 5:FA:252:SER:O | 5:FA:255:ARG:HB2 | 2.12 | 0.49 |
| 5:FA:395:THR:HG22 | 5:FA:396:LYS:H | 1.77 | 0.49 |
| 5:EJ:399:ILE:HD13 | 5:FA:399:ILE:HG22 | 1.94 | 0.49 |
| 5:EI:49:TRP:C | 5:FA:90:ASN:HD21 | 2.10 | 0.49 |
| 6:FD:122:ALA:O | 6:FD:126:VAL:HG23 | 2.12 | 0.49 |
| 7:FE:159:ALA:HB1 | 7:FF:159:ALA:HB2 | 1.94 | 0.49 |
| 7:FF:382:ARG:HG3 | 7:FF:383:TYR:CD2 | 2.47 | 0.49 |
| 7:FE:509:GLY:HA3 | 7:FF:441:GLN:NE2 | 2.27 | 0.49 |
| 7:FE:513:ARG:N | 7:FF:441:GLN:O | 2.32 | 0.49 |
| 7:FG:134:SER:H | 7:FG:142:ILE:HD11 | 1.78 | 0.49 |
| 8:FH:137:VAL:HA | 8:FH:155:VAL:HG12 | 1.94 | 0.49 |
| 8:FI:143:ASP:OD1 | 8:FI:144:TRP:N | 2.45 | 0.49 |
| 12:DJ:153:ARG:NH1 | 12:GC:184:PRO:HA | 2.27 | 0.49 |
| 12:GC:220:SER:HA | 12:GC:243:PHE:CD1 | 2.47 | 0.49 |
| 1:GD:645:ASP:OD1 | 1:GD:645:ASP:N | 2.45 | 0.49 |
| 1:GE:518:ASN:OD1 | 1:GE:535:LEU:HB3 | 2.13 | 0.49 |
| 1:GE:55:VAL:HG21 | 2:GF:657:TYR:CE1 | 2.47 | 0.49 |
| 2:GF:682:GLN:O | 2:GF:685:ASN:HB3 | 2.12 | 0.49 |
| 3:GH:61:PRO:HG3 | 3:GH:314:ASN:OD1 | 2.12 | 0.49 |
| 4:GJ:193:HIS:HA | 4:GJ:260:TYR:HD1 | 1.77 | 0.49 |
| 5:HB:110:VAL:HG22 | 5:HB:123:PRO:HB3 | 1.94 | 0.49 |
| 5:HB:275:SER:OG | 5:HB:282:VAL:HG12 | 2.13 | 0.49 |
| 6:HG:30:MET:O | 6:HG:32:ARG:HG2 | 2.13 | 0.49 |
| 7:HH:160:MET:SD | 7:HH:165:THR:HB | 2.52 | 0.49 |
| 7:HH:503:ASN:OD1 | 7:HJ:446:LYS:N | 2.46 | 0.49 |
| 7:HH:289:GLN:HB2 | 7:HI:286:ASP:O | 2.13 | 0.49 |
| 7:HI:429:CYS:HG | 7:HJ:515:TRP:HE1 | 1.60 | 0.49 |
| 7:HH:407:SER:N | 7:HJ:394:ASP:OD2 | 2.38 | 0.49 |
| 7:HH:42:ALA:HB3 | 7:HJ:43:GLY:O | 2.13 | 0.49 |
| 7:HJ:73:THR:HG23 | 7:HJ:74:LYS:H | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:454:TYR:CD1 | 5:I:458:THR:HG21 | 2.47 | 0.49 |
| 11:IE:2:LEU:O | 11:IE:4:THR:N | 2.45 | 0.49 |
| 5:K:469:PRO:O | 5:K:473:MET:N | 2.45 | 0.49 |
| 7:O:170:ILE:HA | 7:O:173:ILE:HG22 | 1.95 | 0.49 |
| 7:O:263:VAL:O | 7:P:255:SER:OG | 2.15 | 0.49 |
| 5:I:239:GLY:O | 7:O:2:SER:N | 2.46 | 0.49 |
| 7:O:480:ARG:NE | 7:P:465:ARG:HG3 | 2.28 | 0.49 |
| 7:O:61:PRO:HD3 | 7:O:74:LYS:HB3 | 1.95 | 0.49 |
| 7:Q:29:ILE:HG22 | 7:Q:30:THR:N | 2.18 | 0.49 |
| 7:P:515:TRP:CD1 | 7:Q:440:GLN:HB3 | 2.48 | 0.49 |
| 8:R:143:ASP:OD1 | 8:R:144:TRP:N | 2.45 | 0.49 |
| 11:V:138:ASP:HB3 | 11:V:140:ALA:H | 1.77 | 0.49 |
| 10:U:215:SER:O | 12:W:191:LEU:HD13 | 2.13 | 0.49 |
| 1:X:111:MET:SD | 1:X:304:PRO:HB3 | 2.52 | 0.49 |
| 1:X:353:PHE:HD2 | 1:X:392:ILE:HD13 | 1.76 | 0.49 |
| 1:Y:392:ILE:HG23 | 1:Y:408:ILE:HD13 | 1.94 | 0.49 |
| 13:YA:16[E]:GLU:CD | 13:YA:30[E]:ARG:HH11 | 2.16 | 0.49 |
| 13:YA:522[F]:VAL:HG11 | 13:YA:526[F]:GLN:NE2 | 2.27 | 0.49 |
| 13:YB:436[B]:ASP:OD2 | 13:YB:437[B]:ASN:N | 2.45 | 0.49 |
| 13:YB:490[A]:VAL:HG11 | 13:YC:486[A]:GLU:CB | 2.42 | 0.49 |
| 13:YB:538[B]:VAL:HA | 13:YC:530[B]:VAL:O | 2.12 | 0.49 |
| 13:YB:538[E]:VAL:HA | 13:YC:530[E]:VAL:O | 2.12 | 0.49 |
| 13:YB:57[E]:VAL:HG21 | 13:YB:75[E]:GLY:HA2 | 1.94 | 0.49 |
| 13:YA:95[D]:ILE:HD11 | 13:YB:83[D]:TYR:CZ | 2.48 | 0.49 |
| 13:YA:452[E]:GLY:CA | 13:YC:321[E]:LYS:HD3 | 2.40 | 0.49 |
| 13:YB:292[A]:PHE:CD1 | 13:YC:364[A]:ALA:HB2 | 2.47 | 0.49 |
| 13:YA:546[C]:VAL:O | 13:YC:554[C]:MET:HA | 2.13 | 0.49 |
| 13:YA:546[D]:VAL:O | 13:YC:554[D]:MET:HA | 2.13 | 0.49 |
| 13:YA:546[E]:VAL:O | 13:YC:554[E]:MET:HA | 2.13 | 0.49 |
| 13:YA:557[B]:MET:HG2 | 13:YC:565[B]:TYR:CZ | 2.47 | 0.49 |
| 14:YD:184[B]:LYS:HE3 | 14:YD:367[B]:ILE:CG2 | 2.42 | 0.49 |
| 13:YA:24[F]:LEU:HD23 | 14:YD:259[F]:LEU:CD2 | 2.43 | 0.49 |
| 14:YD:301[B]:MET:HA | 14:YD:304[B]:TYR:CD2 | 2.47 | 0.49 |
| 14:YD:360[D]:ASN:ND2 | 14:YD:360[D]:ASN:H | 2.04 | 0.49 |
| 14:YD:373[E]:LYS:HG2 | 14:YD:374[E]:ASN:N | 2.26 | 0.49 |
| 14:YD:47[D]:ARG:O | 14:YD:48[D]:ASN:ND2 | 2.45 | 0.49 |
| 14:YD:47[F]:ARG:O | 14:YD:48[F]:ASN:ND2 | 2.46 | 0.49 |
| 14:YD:72[F]:ILE:O | 14:YD:86[F]:ARG:N | 2.46 | 0.49 |
| 14:YE:301[D]:MET:HA | 14:YE:304[D]:TYR:CD2 | 2.47 | 0.49 |
| 1:A:287:SER:HB2 | 14:YE:373[E]:LYS:HD2 | 1.95 | 0.49 |
| 1:X:130:ARG:HD3 | 14:YF:181[D]:GLY:HA2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:103:PHE:CE2 | 2:Z:627:GLU:HA | 2.48 | 0.49 |
| 2:Z:926:PRO:HG2 | 2:Z:985:GLU:HG2 | 1.94 | 0.49 |
| 15:ZA:29[F]:VAL:HG21 | 15:ZA:69[F]:VAL:HG13 | 1.94 | 0.49 |
| 15:ZA:31[E]:THR:OG1 | 15:ZA:94[E]:VAL:HG21 | 2.12 | 0.49 |
| 1:A:63:ASN:O | 1:A:66:TYR:N | 2.46 | 0.49 |
| 4:AA:70:HIS:HB2 | 4:AA:75:TYR:CE2 | 2.47 | 0.49 |
| 4:AB:194:ARG:HE | 4:AB:259:ASN:HA | 1.78 | 0.49 |
| 5:AC:52:TYR:CZ | 5:AC:60:LEU:HB3 | 2.48 | 0.49 |
| 5:AD:58:GLN:N | 5:AD:58:GLN:OE1 | 2.42 | 0.49 |
| 5:AE:186:TYR:HE1 | 5:AE:246:THR:HA | 1.78 | 0.49 |
| 5:AD:319:GLU:HG3 | 5:AE:262:GLN:OE1 | 2.13 | 0.49 |
| 6:AH:30:MET:O | 6:AH:32:ARG:HG2 | 2.13 | 0.49 |
| 7:AI:100:TYR:CZ | 7:AJ:113:GLU:HA | 2.48 | 0.49 |
| 1:B:19:GLU:O | 1:B:19:GLU:HG2 | 2.13 | 0.49 |
| 7:BA:325:TYR:CD1 | 7:BA:330:ARG:HA | 2.45 | 0.49 |
| 7:AI:42:ALA:HB3 | 7:BA:43:GLY:O | 2.13 | 0.49 |
| 11:BF:124:ILE:HG22 | 11:BF:135:ASP:O | 2.13 | 0.49 |
| 12:BG:31:SER:O | 12:BG:32:THR:OG1 | 2.30 | 0.49 |
| 1:BH:539:ARG:CD | 1:BH:580:LEU:HD23 | 2.42 | 0.49 |
| 1:BI:370:GLY:C | 1:BI:404:ILE:HG13 | 2.33 | 0.49 |
| 2:BJ:191:TYR:CE1 | 2:BJ:235:LYS:HA | 2.47 | 0.49 |
| 2:BJ:444:SER:HB2 | 2:BJ:512:PRO:HG3 | 1.94 | 0.49 |
| 2:BJ:173:TYR:CE1 | 2:BJ:579:LYS:HE2 | 2.47 | 0.49 |
| 2:BJ:103:PHE:CE2 | 2:BJ:627:GLU:HA | 2.48 | 0.49 |
| 2:C:191:TYR:CE1 | 2:C:235:LYS:HA | 2.47 | 0.49 |
| 2:C:253:ILE:HG13 | 2:C:300:LEU:HD21 | 1.94 | 0.49 |
| 4:CD:194:ARG:HE | 4:CD:259:ASN:HA | 1.78 | 0.49 |
| 5:CF:359:GLU:H | 5:CF:370:HIS:C | 2.15 | 0.49 |
| 5:CG:102:TRP:HB2 | 5:CG:129:ARG:O | 2.12 | 0.49 |
| 5:CH:186:TYR:HE1 | 5:CH:246:THR:HA | 1.78 | 0.49 |
| 6:CJ:100:PRO:O | 6:CJ:103:SER:OG | 2.18 | 0.49 |
| 7:DB:451:PHE:CD1 | 7:DB:469:VAL:HG13 | 2.48 | 0.49 |
| 7:DB:14:ARG:NH2 | 7:DC:19:ASP:OD2 | 2.44 | 0.49 |
| 7:DD:196:VAL:HA | 7:DD:199:VAL:HG22 | 1.95 | 0.49 |
| 7:DD:63:GLU:OE1 | 7:DD:80:THR:HA | 2.13 | 0.49 |
| 8:DE:137:VAL:HA | 8:DE:155:VAL:HG12 | 1.93 | 0.49 |
| 8:DE:143:ASP:OD1 | 8:DE:144:TRP:N | 2.45 | 0.49 |
| 2:EC:1003:GLN:OE1 | 5:EI:10:VAL:HA | 2.12 | 0.49 |
| 2:EC:253:ILE:HG13 | 2:EC:300:LEU:HD21 | 1.94 | 0.49 |
| 2:EC:453:ASP:HB3 | 2:EC:474:GLU:O | 2.12 | 0.49 |
| 4:F:79:VAL:N | 4:F:97:ILE:O | 2.32 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:196:ARG:HG2 | 5:FA:198:ASN:O | 2.12 | 0.49 |
| 7:FE:349:TRP:CZ3 | 7:FF:342:PRO:HG2 | 2.47 | 0.49 |
| 7:FF:515:TRP:CD1 | 7:FG:440:GLN:HB3 | 2.48 | 0.49 |
| 7:FG:171:LYS:O | 7:FG:175:GLN:HG3 | 2.13 | 0.49 |
| 7:FG:405:ARG:NH2 | 7:FG:409:LEU:O | 2.46 | 0.49 |
| 1:GD:12:ARG:O | 2:GF:709:TYR:OH | 2.23 | 0.49 |
| 1:GE:209:TRP:CZ3 | 1:GE:212:LYS:NZ | 2.69 | 0.49 |
| 2:GF:319:TYR:CD1 | 2:GF:328:TYR:HB2 | 2.47 | 0.49 |
| 2:GF:357:ILE:HG12 | 2:GF:358:THR:H | 1.77 | 0.49 |
| 2:GF:926:PRO:HG2 | 2:GF:985:GLU:HG2 | 1.94 | 0.49 |
| 3:GG:279:LEU:HD12 | 3:GH:232:GLN:HE21 | 1.77 | 0.49 |
| 3:GG:50:ASN:HB2 | 3:GG:56:PHE:CE1 | 2.47 | 0.49 |
| 3:GH:3:ASP:OD1 | 3:GH:4:SER:N | 2.45 | 0.49 |
| 4:GI:194:ARG:HE | 4:GI:259:ASN:HA | 1.78 | 0.49 |
| 4:GI:193:HIS:HA | 4:GI:260:TYR:HD1 | 1.77 | 0.49 |
| 4:GJ:139:VAL:HG21 | 4:GJ:146:VAL:HG21 | 1.94 | 0.49 |
| 4:HA:194:ARG:HE | 4:HA:259:ASN:HA | 1.78 | 0.49 |
| 5:HB:563:GLY:HA3 | 5:HB:566:TYR:OH | 2.12 | 0.49 |
| 5:HC:240:ASP:OD1 | 7:HJ:4:ASN:ND2 | 2.46 | 0.49 |
| 5:HC:168:LEU:HA | 5:HC:241:THR:HG22 | 1.94 | 0.49 |
| 7:HH:134:SER:HB3 | 7:HH:140:GLY:N | 2.28 | 0.49 |
| 5:I:407:TYR:HD2 | 5:J:407:TYR:CE2 | 2.31 | 0.49 |
| 5:I:506:LEU:HB3 | 5:I:510:GLY:HA2 | 1.93 | 0.49 |
| 5:I:563:GLY:HA3 | 5:I:566:TYR:OH | 2.12 | 0.49 |
| 11:IE:124:ILE:HG22 | 11:IE:135:ASP:O | 2.13 | 0.49 |
| 12:IF:178:VAL:O | 12:IF:181:VAL:HG12 | 2.13 | 0.49 |
| 5:J:312:ARG:HD3 | 5:J:317:LEU:HD12 | 1.93 | 0.49 |
| 5:K:206:PHE:HZ | 5:K:221:GLU:HG2 | 1.76 | 0.49 |
| 5:K:359:GLU:O | 5:K:370:HIS:N | 2.36 | 0.49 |
| 6:M:4:LEU:HD23 | 6:M:5:ASN:N | 2.27 | 0.49 |
| 7:O:106:ALA:HB2 | 7:O:120:LYS:HD2 | 1.94 | 0.49 |
| 7:O:263:VAL:O | 7:P:260:ARG:HA | 2.13 | 0.49 |
| 7:P:120:LYS:O | 7:P:124:ALA:N | 2.46 | 0.49 |
| 7:P:236:VAL:O | 7:P:253:ARG:NH1 | 2.46 | 0.49 |
| 7:O:485:ASN:C | 7:P:446:LYS:HG2 | 2.33 | 0.49 |
| 7:O:202:GLY:HA3 | 7:Q:216:MET:SD | 2.51 | 0.49 |
| 7:Q:338:ASP:HB2 | 7:Q:527:GLU:OE2 | 2.12 | 0.49 |
| 7:Q:405:ARG:NH2 | 7:Q:409:LEU:O | 2.46 | 0.49 |
| 7:P:43:GLY:O | 7:Q:42:ALA:HB3 | 2.13 | 0.49 |
| 7:O:471:THR:HA | 7:Q:474:GLY:O | 2.13 | 0.49 |
| 1:X:378:PRO:HG3 | 1:X:384:LEU:HG | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:321[C]:LYS:HD3 | 13:YB:452[C]:GLY:CA | 2.34 | 0.49 |
| 13:YA:522[D]:VAL:HG11 | 13:YA:526[D]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:538[A]:VAL:HG21 | 13:YB:534[A]:LEU:HD22 | 1.94 | 0.49 |
| 13:YA:67[C]:SER:HB3 | 13:YB:123[C]:ARG:HB2 | 1.95 | 0.49 |
| 13:YA:76[A]:PRO:C | 13:YA:98[A]:GLY:HA2 | 2.33 | 0.49 |
| 13:YB:307[E]:ALA:HB1 | 13:YB:331[E]:ILE:HD11 | 1.95 | 0.49 |
| 13:YB:387[E]:TYR:CE1 | 13:YB:388[E]:PRO:HB3 | 2.48 | 0.49 |
| 13:YB:540[B]:GLY:HA3 | 13:YC:533[B]:ASN:ND2 | 2.22 | 0.49 |
| 13:YB:540[F]:GLY:HA3 | 13:YC:533[F]:ASN:ND2 | 2.22 | 0.49 |
| 13:YB:76[D]:PRO:C | 13:YB:98[D]:GLY:HA2 | 2.33 | 0.49 |
| 13:YC:266[E]:TRP:O | 13:YC:274[E]:GLN:NE2 | 2.46 | 0.49 |
| 13:YC:344[E]:LYS:HA | 13:YC:344[E]:LYS:HE2 | 1.93 | 0.49 |
| 13:YC:522[B]:VAL:HG11 | 13:YC:526[B]:GLN:NE2 | 2.27 | 0.49 |
| 13:YA:123[F]:ARG:HB2 | 13:YC:67[F]:SER:HB3 | 1.95 | 0.49 |
| 13:YA:34[B]:LEU:HD13 | 14:YD:163[B]:THR:HG21 | 1.94 | 0.49 |
| 14:YD:16[E]:LEU:HB2 | 14:YD:70[E]:ILE:HD13 | 1.94 | 0.49 |
| 14:YD:293[F]:GLU:OE1 | 14:YD:293[F]:GLU:N | 2.45 | 0.49 |
| 14:YE:16[E]:LEU:HB2 | 14:YE:70[E]:ILE:HD13 | 1.94 | 0.49 |
| 14:YE:301[F]:MET:HA | 14:YE:304[F]:TYR:CD2 | 2.47 | 0.49 |
| 14:YE:184[C]:LYS:HE3 | 14:YE:367[C]:ILE:CG2 | 2.42 | 0.49 |
| 14:YE:184[F]:LYS:HE3 | 14:YE:367[F]:ILE:CG2 | 2.42 | 0.49 |
| 14:YF:45[D]:TYR:O | 14:YF:174[D]:ARG:NH2 | 2.46 | 0.49 |
| 14:YF:184[D]:LYS:HE3 | 14:YF:367[D]:ILE:CG2 | 2.42 | 0.49 |
| 11:V:190:LYS:HZ1 | 14:YF:24[D]:SER:HA | 1.78 | 0.49 |
| 14:YF:301[D]:MET:HA | 14:YF:304[D]:TYR:CD2 | 2.47 | 0.49 |
| 14:YF:360[D]:ASN:N | 14:YF:360[D]:ASN:HD22 | 1.97 | 0.49 |
| 14:YF:184[C]:LYS:HE3 | 14:YF:367[C]:ILE:CG2 | 2.42 | 0.49 |
| 14:YF:47[C]:ARG:O | 14:YF:48[C]:ASN:ND2 | 2.45 | 0.49 |
| 14:YE:332[D]:GLN:HB3 | 14:YF:61[D]:HIS:NE2 | 2.28 | 0.49 |
| 14:YF:72[B]:ILE:O | 14:YF:86[B]:ARG:N | 2.46 | 0.49 |
| 2:Z:360:ASN:O | 2:Z:362:LYS:HG3 | 2.13 | 0.49 |
| 2:Z:433:ASN:HD21 | 2:Z:513:PHE:HA | 1.75 | 0.49 |
| 2:Z:63:ALA:HB3 | 4:AA:83:THR:HA | 149.15 | 0.49 |
| 1:A:229:THR:OG1 | 1:A:233:ASN:OD1 | 2.30 | 0.49 |
| 4:AA:193:HIS:HA | 4:AA:260:TYR:HD1 | 1.77 | 0.49 |
| 5:AC:20:ARG:HH12 | 5:AC:24:ILE:HD12 | 1.78 | 0.49 |
| 5:AC:291:ILE:HG22 | 5:AC:292:PRO:O | 2.13 | 0.49 |
| 5:AC:154:ILE:HG23 | 5:AD:153:LYS:HZ1 | 1.78 | 0.49 |
| 5:AD:2:LYS:H | 5:AE:41:ASP:HB3 | 1.77 | 0.49 |
| 5:AE:469:PRO:O | 5:AE:473:MET:N | 2.45 | 0.49 |
| 7:AI:163:LEU:O | 7:AI:167:GLN:N | 2.25 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:161:THR:O | 7:AI:165:THR:HG22 | 2.13 | 0.49 |
| 7:AI:176:ILE:HG23 | 7:AI:177:ALA:N | 2.28 | 0.49 |
| 7:AI:503:ASN:OD1 | 7:BA:446:LYS:N | 2.46 | 0.49 |
| 7:AI:504:ARG:HA | 7:BA:422:LYS:HB3 | 1.95 | 0.49 |
| 7:AJ:43:GLY:O | 7:BA:42:ALA:HB3 | 2.13 | 0.49 |
| 7:BA:134:SER:H | 7:BA:142:ILE:HD11 | 1.78 | 0.49 |
| 7:AJ:227:VAL:HG23 | 7:BA:225:LYS:HD3 | 1.95 | 0.49 |
| 9:BD:18:ASP:OD1 | 9:BD:19:TRP:N | 2.46 | 0.49 |
| 10:BE:285:LEU:HA | 14:YD:215[C]:GLU:HG3 | 1.92 | 0.49 |
| 10:BE:313:PRO:HG2 | 10:BE:351:ILE:HG22 | 1.93 | 0.49 |
| 1:BH:430:GLN:N | 1:BH:430:GLN:OE1 | 2.29 | 0.49 |
| 1:BH:647:ARG:HH11 | 1:BH:650:TYR:HE2 | 1.60 | 0.49 |
| 1:BI:114:CYS:SG | 1:BI:295:ILE:HG23 | 2.53 | 0.49 |
| 1:BI:209:TRP:HE3 | 1:BI:212:LYS:CB | 2.26 | 0.49 |
| 2:BJ:221:ALA:O | 5:CG:564:PRO:HG2 | 2.12 | 0.49 |
| 2:BJ:453:ASP:HB3 | 2:BJ:474:GLU:O | 2.13 | 0.49 |
| 2:C:341:LEU:O | 2:C:342:SER:HB2 | 2.13 | 0.49 |
| 4:CD:193:HIS:HA | 4:CD:260:TYR:HD1 | 1.77 | 0.49 |
| 4:CE:70:HIS:HB2 | 4:CE:75:TYR:CE2 | 2.47 | 0.49 |
| 5:CF:290:SER:CB | 5:CF:371:PHE:H | 2.26 | 0.49 |
| 5:CG:202:TYR:OH | 5:CG:223:VAL:O | 2.18 | 0.49 |
| 6:DA:30:MET:O | 6:DA:32:ARG:HG2 | 2.13 | 0.49 |
| 7:DC:14:ARG:HG2 | 7:DC:33:GLN:HG2 | 1.93 | 0.49 |
| 7:DC:151:LEU:HD12 | 7:DC:171:LYS:HE2 | 1.95 | 0.49 |
| 7:DC:35:ALA:O | 7:DC:39:ILE:HD12 | 2.13 | 0.49 |
| 7:DC:54:THR:HG22 | 7:DC:55:LYS:O | 2.13 | 0.49 |
| 7:DD:29:ILE:HG22 | 7:DD:30:THR:N | 2.18 | 0.49 |
| 7:DD:386:ASN:HB2 | 7:DD:387:PRO:HD2 | 1.94 | 0.49 |
| 7:DD:405:ARG:NH2 | 7:DD:409:LEU:O | 2.46 | 0.49 |
| 1:BI:65:LEU:HD21 | 11:DI:70:TYR:OH | 2.13 | 0.49 |
| 1:EA:512:SER:OG | 1:EA:513:ASN:N | 2.44 | 0.49 |
| 1:EB:370:GLY:C | 1:EB:404:ILE:HG13 | 2.33 | 0.49 |
| 2:EC:103:PHE:CE2 | 2:EC:627:GLU:HA | 2.48 | 0.49 |
| 2:EC:173:TYR:CE1 | 2:EC:579:LYS:HE2 | 2.47 | 0.49 |
| 2:EC:234:SER:OG | 2:EC:366:TYR:O | 2.25 | 0.49 |
| 3:ED:233:GLN:HB2 | 3:EE:289:ASN:HD21 | 1.78 | 0.49 |
| 4:EG:111:ASN:HD21 | 4:EG:115:SER:N | 2.10 | 0.49 |
| 4:EF:4:GLN:NE2 | 4:EH:61:ILE:O | 2.41 | 0.49 |
| 5:EI:149:LYS:HG2 | 5:EI:150:GLN:N | 2.27 | 0.49 |
| 2:EC:976:SER:HB2 | 5:EJ:10:VAL:HG21 | 1.94 | 0.49 |
| 5:EJ:19:LEU:HD13 | 5:FA:19:LEU:HD21 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:323:THR:CG2 | 5:FA:354:THR:HG23 | 2.42 | 0.49 |
| 5:FA:358:VAL:HG23 | 5:FA:371:PHE:HD1 | 1.78 | 0.49 |
| 5:FA:501:LEU:HB3 | 5:FA:512:PRO:HB2 | 1.94 | 0.49 |
| 7:FG:118:PRO:O | 7:FG:122:THR:N | 2.41 | 0.49 |
| 7:FG:338:ASP:HB2 | 7:FG:527:GLU:OE2 | 2.12 | 0.49 |
| 7:FG:65:GLU:O | 7:FG:69:GLY:N | 2.46 | 0.49 |
| 7:FG:73:THR:HG23 | 7:FG:74:LYS:H | 1.78 | 0.49 |
| 8:FH:10:PHE:CE2 | 8:FH:15:PHE:CE1 | 3.01 | 0.49 |
| 1:EB:52:ARG:HE | 9:FJ:13:PRO:HB3 | 1.78 | 0.49 |
| 12:GC:178:VAL:O | 12:GC:181:VAL:HG12 | 2.13 | 0.49 |
| 12:GC:158:LEU:HD21 | 12:GC:216:PHE:CE1 | 2.48 | 0.49 |
| 1:GD:635:ARG:NH2 | 3:GH:322:MET:SD | 2.82 | 0.49 |
| 1:GD:377:LYS:CD | 1:GD:641:VAL:HG21 | 2.43 | 0.49 |
| 1:GE:229:THR:OG1 | 1:GE:231:ASP:OD1 | 2.31 | 0.49 |
| 1:GE:627:PRO:HG3 | 1:GE:632:ILE:HD11 | 1.94 | 0.49 |
| 2:GF:1000:THR:HG23 | 5:HB:17:ASP:O | 2.12 | 0.49 |
| 2:GF:1005:ARG:HG3 | 5:HB:12:ASP:OD2 | 2.12 | 0.49 |
| 3:GG:31:GLY:O | 3:GG:291:LYS:NZ | 2.31 | 0.49 |
| 3:GG:43:ARG:N | 3:GG:74:HIS:HB3 | 2.28 | 0.49 |
| 2:EC:507:LYS:O | 3:GH:176:ALA:HB2 | 2.13 | 0.49 |
| 4:GJ:79:VAL:N | 4:GJ:97:ILE:O | 2.32 | 0.49 |
| 4:H:194:ARG:HE | 4:H:259:ASN:HA | 1.78 | 0.49 |
| 4:HA:111:ASN:HD21 | 4:HA:115:SER:N | 2.10 | 0.49 |
| 5:HB:20:ARG:HH12 | 5:HB:24:ILE:HD12 | 1.78 | 0.49 |
| 5:HC:267:ASP:OD1 | 5:HC:285:LEU:HB2 | 2.12 | 0.49 |
| 5:HB:182:ARG:NH2 | 5:HC:299:ILE:HG21 | 2.27 | 0.49 |
| 5:HD:206:PHE:CG | 5:HD:223:VAL:HA | 2.47 | 0.49 |
| 5:HD:395:THR:HG22 | 5:HD:396:LYS:H | 1.77 | 0.49 |
| 6:HG:122:ALA:O | 6:HG:126:VAL:HG23 | 2.12 | 0.49 |
| 7:HH:482:TYR:OH | 7:HI:453:GLU:HB2 | 2.12 | 0.49 |
| 5:I:194:LYS:O | 5:I:242:VAL:HA | 2.13 | 0.49 |
| 5:I:275:SER:OG | 5:I:282:VAL:HG12 | 2.13 | 0.49 |
| 5:I:285:LEU:HD11 | 5:I:375:PHE:CB | 2.41 | 0.49 |
| 5:I:359:GLU:H | 5:I:370:HIS:C | 2.15 | 0.49 |
| 5:I:264:ARG:HG3 | 5:I:379:ASP:O | 2.10 | 0.49 |
| 8:IA:137:VAL:HA | 8:IA:155:VAL:HG12 | 1.93 | 0.49 |
| 5:J:319:GLU:OE2 | 5:J:324:VAL:HG13 | 2.13 | 0.49 |
| 5:K:320:LEU:HB3 | 5:K:358:VAL:HB | 1.95 | 0.49 |
| 5:K:358:VAL:HG23 | 5:K:371:PHE:HD1 | 1.78 | 0.49 |
| 5:I:569:TYR:CE2 | 5:K:542:LEU:HD11 | 2.48 | 0.49 |
| 6:M:73:ASN:HD21 | 6:M:215:PHE:HE2 | 1.59 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:117:THR:CB | 7:Q:112:ASN:HA | 2.43 | 0.49 |
| 7:P:14:ARG:HG2 | 7:P:33:GLN:HG2 | 1.93 | 0.49 |
| 7:P:371:ASP:OD1 | 7:P:526:LYS:NZ | 2.45 | 0.49 |
| 7:P:382:ARG:HG3 | 7:P:383:TYR:CD2 | 2.47 | 0.49 |
| 7:O:140:GLY:O | 7:Q:141:VAL:HG23 | 2.13 | 0.49 |
| 8:S:31:ASN:HA | 1:Y:76:TYR:CE2 | 189.61 | 0.49 |
| 12:W:158:LEU:HD21 | 12:W:216:PHE:CE1 | 2.48 | 0.49 |
| 12:W:184:PRO:HA | 12:IF:153:ARG:NH1 | 2.27 | 0.49 |
| 12:W:99:SER:HB2 | 12:IF:215:MET:HE1 | 1.94 | 0.49 |
| 1:X:339:CYS:HA | 1:X:344:ASP:OD2 | 2.13 | 0.49 |
| 1:Y:209:TRP:HE3 | 1:Y:212:LYS:CB | 2.26 | 0.49 |
| 1:Y:114:CYS:SG | 1:Y:295:ILE:HG23 | 2.52 | 0.49 |
| 1:Y:526:PRO:HB2 | 1:Y:528:THR:HG23 | 1.94 | 0.49 |
| 13:YA:12[B]:VAL:HG21 | 14:YF:256[B]:HIS:CE1 | 2.47 | 0.49 |
| 13:YA:95[C]:ILE:HD11 | 13:YB:83[C]:TYR:CZ | 2.48 | 0.49 |
| 13:YB:109[D]:ASN:HB3 | 13:YB:112[D]:GLU:HB2 | 1.94 | 0.49 |
| 13:YB:522[D]:VAL:HG11 | 13:YB:526[D]:GLN:NE2 | 2.27 | 0.49 |
| 13:YB:292[E]:PHE:CD1 | 13:YC:364[E]:ALA:HB2 | 2.48 | 0.49 |
| 13:YB:490[F]:VAL:HG11 | 13:YC:486[F]:GLU:CB | 2.43 | 0.49 |
| 13:YB:538[A]:VAL:HA | 13:YC:530[A]:VAL:O | 2.12 | 0.49 |
| 13:YA:122[B]:PRO:HB3 | 13:YC:66[B]:MET:HE2 | 1.95 | 0.49 |
| 14:YD:184[A]:LYS:HE3 | 14:YD:367[A]:ILE:CG2 | 2.42 | 0.49 |
| 11:V:190:LYS:HZ1 | 14:YD:24[B]:SER:HA | 1.78 | 0.49 |
| 13:YB:44[C]:VAL:HG11 | 14:YD:272[C]:GLU:HB3 | 1.94 | 0.49 |
| 14:YD:301[A]:MET:HA | 14:YD:304[A]:TYR:CD2 | 2.47 | 0.49 |
| 14:YD:304[B]:TYR:HB3 | 14:YD:358[B]:PHE:HD1 | 1.78 | 0.49 |
| 14:YD:360[B]:ASN:N | 14:YD:360[B]:ASN:HD22 | 1.98 | 0.49 |
| 1:BH:287:SER:HB2 | 14:YD:373[D]:LYS:HD2 | 1.95 | 0.49 |
| 14:YD:54[A]:PHE:CZ | 14:YD:105[A]:ILE:HD11 | 2.48 | 0.49 |
| 14:YE:16[D]:LEU:HB2 | 14:YE:70[D]:ILE:HD13 | 1.94 | 0.49 |
| 14:YE:252[E]:THR:OG1 | 14:YE:271[E]:GLY:O | 2.31 | 0.49 |
| 14:YE:301[E]:MET:HA | 14:YE:304[E]:TYR:CD2 | 2.47 | 0.49 |
| 14:YE:47[B]:ARG:O | 14:YE:48[B]:ASN:ND2 | 2.45 | 0.49 |
| 14:YE:47[E]:ARG:O | 14:YE:48[E]:ASN:ND2 | 2.45 | 0.49 |
| 10:GA:285:LEU:HA | 14:YF:215[A]:GLU:HG3 | 1.93 | 0.49 |
| 14:YF:252[E]:THR:OG1 | 14:YF:271[E]:GLY:O | 2.31 | 0.49 |
| 14:YF:301[C]:MET:HA | 14:YF:304[C]:TYR:CD2 | 2.47 | 0.49 |
| 14:YF:54[B]:PHE:CZ | 14:YF:105[B]:ILE:HD11 | 2.48 | 0.49 |
| 14:YF:16[D]:LEU:HB2 | 14:YF:70[D]:ILE:HD13 | 1.93 | 0.49 |
| 14:YF:72[F]:ILE:O | 14:YF:86[F]:ARG:N | 2.46 | 0.49 |
| 2:Z:314:THR:CG2 | 2:Z:317:TYR:HB2 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:321:VAL:HB | 2:Z:326:VAL:HG12 | 1.94 | 0.49 |
| 2:Z:357:ILE:HG12 | 2:Z:358:THR:H | 1.77 | 0.49 |
| 2:Z:453:ASP:HB3 | 2:Z:474:GLU:O | 2.12 | 0.49 |
| 2:Z:174:HIS:CG | 2:Z:508:TYR:HH | 2.28 | 0.49 |
| 2:Z:6:PRO:O | 2:Z:7:SER:OG | 2.27 | 0.49 |
| 15:ZA:29[A]:VAL:HG21 | 15:ZA:69[A]:VAL:HG13 | 1.95 | 0.49 |
| 5:AC:454:TYR:CD1 | 5:AC:458:THR:HG21 | 2.47 | 0.49 |
| 5:AC:89:TYR:O | 5:AC:91:LYS:HG2 | 2.13 | 0.49 |
| 5:AD:147:LYS:HE2 | 5:AD:155:THR:HB | 1.94 | 0.49 |
| 5:AE:170:GLU:O | 5:AE:171:VAL:HG12 | 2.13 | 0.49 |
| 6:AF:30:MET:O | 6:AF:32:ARG:HG2 | 2.13 | 0.49 |
| 6:AG:10:VAL:HG22 | 6:AH:13:ARG:HB2 | 1.95 | 0.49 |
| 7:AJ:511:GLU:HB3 | 7:AJ:513:ARG:HH11 | 1.78 | 0.49 |
| 1:B:370:GLY:C | 1:B:404:ILE:HG13 | 2.33 | 0.49 |
| 1:B:45:ASP:C | 1:B:47:ASP:H | 2.10 | 0.49 |
| 1:B:619:GLN:N | 1:B:619:GLN:OE1 | 2.35 | 0.49 |
| 7:AI:399:PHE:HD2 | 7:BA:514:PRO:HG2 | 1.77 | 0.49 |
| 12:BG:153:ARG:NH1 | 12:DJ:184:PRO:HA | 2.27 | 0.49 |
| 10:BE:330:ASN:HB2 | 12:BG:189:ARG:NH2 | 2.28 | 0.49 |
| 1:BI:117:ALA:HB3 | 1:BI:294:ASN:HA | 1.95 | 0.49 |
| 2:BJ:250:TYR:CZ | 2:BJ:306:ARG:HD3 | 2.48 | 0.49 |
| 2:BJ:319:TYR:CD1 | 2:BJ:328:TYR:HB2 | 2.47 | 0.49 |
| 2:BJ:336:ILE:O | 2:BJ:348:ARG:HB2 | 2.12 | 0.49 |
| 2:C:186:ASP:HB3 | 2:C:189:ARG:NE | 2.28 | 0.49 |
| 2:C:221:ALA:H | 5:J:562:SER:CB | 2.25 | 0.49 |
| 2:C:20:GLN:HG2 | 2:C:70:ASP:CG | 2.33 | 0.49 |
| 4:CC:194:ARG:HE | 4:CC:259:ASN:HA | 1.78 | 0.49 |
| 4:CC:79:VAL:N | 4:CC:97:ILE:O | 2.32 | 0.49 |
| 5:CF:89:TYR:O | 5:CF:91:LYS:HG2 | 2.13 | 0.49 |
| 5:CG:416:ILE:O | 5:CG:438:SER:HA | 2.13 | 0.49 |
| 5:CH:170:GLU:O | 5:CH:171:VAL:HG12 | 2.13 | 0.49 |
| 5:CH:188:VAL:HG23 | 5:CH:225:LEU:HD22 | 1.95 | 0.49 |
| 3:D:43:ARG:N | 3:D:74:HIS:HB3 | 2.28 | 0.49 |
| 7:DB:493:GLU:HA | 7:DB:496:ARG:NH2 | 2.28 | 0.49 |
| 7:DC:236:VAL:O | 7:DC:253:ARG:NH1 | 2.46 | 0.49 |
| 7:DC:43:GLY:O | 7:DD:42:ALA:HB3 | 2.12 | 0.49 |
| 7:DC:515:TRP:CD1 | 7:DD:440:GLN:HB3 | 2.48 | 0.49 |
| 9:DG:18:ASP:OD1 | 9:DG:19:TRP:N | 2.46 | 0.49 |
| 12:BG:16:PHE:N | 12:DJ:166:SER:OG | 2.46 | 0.49 |
| 1:EB:506:LYS:O | 1:EB:509:SER:OG | 2.19 | 0.49 |
| 2:EC:248:LEU:HG | 2:EC:311:ILE:CG1 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:909:THR:HG23 | 2:EC:910:GLU:H | 1.77 | 0.49 |
| 2:BJ:454:ASN:ND2 | 3:ED:47:TRP:HB2 | 2.28 | 0.49 |
| 4:EF:194:ARG:HE | 4:EF:259:ASN:HA | 1.78 | 0.49 |
| 4:EH:194:ARG:HE | 4:EH:259:ASN:HA | 1.78 | 0.49 |
| 4:EH:70:HIS:HB2 | 4:EH:75:TYR:CE2 | 2.47 | 0.49 |
| 5:FA:148:ASN:OD1 | 5:FA:149:LYS:N | 2.46 | 0.49 |
| 6:FB:147:LYS:O | 6:FB:157:GLU:N | 2.44 | 0.49 |
| 6:FB:30:MET:O | 6:FB:32:ARG:HG2 | 2.13 | 0.49 |
| 6:FC:30:MET:O | 6:FC:32:ARG:HG2 | 2.13 | 0.49 |
| 7:FE:146:SER:N | 7:FF:136:GLU:OE1 | 2.45 | 0.49 |
| 7:FE:43:GLY:HA3 | 7:FF:39:ILE:HG23 | 1.95 | 0.49 |
| 7:FG:125:LEU:O | 7:FG:129:PHE:N | 2.40 | 0.49 |
| 1:GD:448:TYR:HA | 1:GD:452:VAL:HG12 | 1.95 | 0.49 |
| 1:GE:117:ALA:HB3 | 1:GE:294:ASN:HA | 1.95 | 0.49 |
| 2:GF:186:ASP:HB3 | 2:GF:189:ARG:NE | 2.28 | 0.49 |
| 2:GF:314:THR:CG2 | 2:GF:317:TYR:HB2 | 2.43 | 0.49 |
| 4:GI:107:VAL:O | 4:GI:148:LEU:N | 2.39 | 0.49 |
| 4:F:7:LYS:NZ | 4:H:36:ASN:OD1 | 2.27 | 0.49 |
| 5:HB:291:ILE:HG22 | 5:HB:292:PRO:O | 2.13 | 0.49 |
| 5:HB:7:ILE:HG12 | 5:HC:24:ILE:HG13 | 1.95 | 0.49 |
| 5:HC:147:LYS:HE2 | 5:HC:155:THR:HB | 1.94 | 0.49 |
| 5:HC:305:ASN:HB3 | 5:HD:255:ARG:HH12 | 1.78 | 0.49 |
| 5:HC:335:ASP:N | 5:HC:335:ASP:OD1 | 2.45 | 0.49 |
| 5:HD:117:ILE:HA | 5:HD:143:TRP:HB2 | 1.94 | 0.49 |
| 7:HH:100:TYR:CZ | 7:HI:113:GLU:HA | 2.48 | 0.49 |
| 7:HH:170:ILE:HA | 7:HH:173:ILE:HG22 | 1.95 | 0.49 |
| 7:HI:117:THR:CB | 7:HJ:112:ASN:HA | 2.42 | 0.49 |
| 7:HJ:87:TYR:HD1 | 7:HJ:88:PRO:O | 1.96 | 0.49 |
| 5:I:290:SER:CB | 5:I:371:PHE:H | 2.26 | 0.49 |
| 5:I:97:ASP:HB3 | 5:I:99:PHE:O | 2.13 | 0.49 |
| 5:J:416:ILE:O | 5:J:438:SER:HA | 2.13 | 0.49 |
| 5:I:568:LYS:HA | 5:J:550:VAL:O | 2.12 | 0.49 |
| 5:K:196:ARG:HD2 | 7:P:5:THR:OG1 | 2.13 | 0.49 |
| 5:J:313:PHE:HE1 | 6:L:8:ALA:HB1 | 1.78 | 0.49 |
| 6:N:30:MET:O | 6:N:32:ARG:HG2 | 2.13 | 0.49 |
| 7:O:479:ASN:O | 7:P:468:PHE:HB2 | 2.13 | 0.49 |
| 7:O:493:GLU:HA | 7:O:496:ARG:NH2 | 2.28 | 0.49 |
| 7:P:227:VAL:HG23 | 7:Q:225:LYS:HD3 | 1.95 | 0.49 |
| 11:V:146:TYR:CE2 | 11:V:150:LEU:HD23 | 2.48 | 0.49 |
| 1:X:411:PRO:HG2 | 1:X:413:TYR:HD2 | 1.77 | 0.49 |
| 1:X:424:TYR:OH | 1:X:657:PRO:HG3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:370:GLY:C | 1:Y:404:ILE:HG13 | 2.33 | 0.49 |
| 1:Y:55:VAL:HG21 | 2:Z:657:TYR:CE1 | 2.48 | 0.49 |
| 13:YA:266[F]:TRP:O | 13:YA:274[F]:GLN:NE2 | 2.46 | 0.49 |
| 13:YA:307[A]:ALA:HB1 | 13:YA:331[A]:ILE:HD11 | 1.95 | 0.49 |
| 13:YA:344[C]:LYS:HA | 13:YA:344[C]:LYS:HE2 | 1.94 | 0.49 |
| 13:YA:407[A]:PRO:HB3 | 13:YC:232[A]:ASN:HB3 | 1.94 | 0.49 |
| 13:YA:66[E]:MET:O | 13:YA:69[E]:ILE:N | 2.46 | 0.49 |
| 13:YA:474[B]:ILE:HG12 | 13:YB:466[B]:ASN:HB2 | 1.93 | 0.49 |
| 13:YC:109[F]:ASN:HB3 | 13:YC:112[F]:GLU:HB2 | 1.95 | 0.49 |
| 13:YC:16[B]:GLU:CD | 13:YC:30[B]:ARG:HH11 | 2.16 | 0.49 |
| 13:YC:16[C]:GLU:CD | 13:YC:30[C]:ARG:HH11 | 2.17 | 0.49 |
| 13:YA:407[C]:PRO:HB3 | 13:YC:232[C]:ASN:HB3 | 1.94 | 0.49 |
| 13:YC:76[D]:PRO:C | 13:YC:98[D]:GLY:HA2 | 2.33 | 0.49 |
| 14:YE:360[F]:ASN:HD22 | 14:YE:360[F]:ASN:N | 1.98 | 0.49 |
| 14:YE:72[A]:ILE:O | 14:YE:86[A]:ARG:N | 2.46 | 0.49 |
| 13:YC:34[A]:LEU:HD13 | 14:YF:163[A]:THR:HG21 | 1.94 | 0.49 |
| 14:YF:16[A]:LEU:HB2 | 14:YF:70[A]:ILE:HD13 | 1.94 | 0.49 |
| 14:YF:16[F]:LEU:HB2 | 14:YF:70[F]:ILE:HD13 | 1.94 | 0.49 |
| 14:YF:301[E]:MET:HA | 14:YF:304[E]:TYR:CD2 | 2.47 | 0.49 |
| 2:Z:191:TYR:CE1 | 2:Z:235:LYS:HA | 2.47 | 0.49 |
| 2:Z:20:GLN:HG2 | 2:Z:70:ASP:CG | 2.33 | 0.49 |
| 1:A:210:THR:HG22 | 1:A:225:TYR:HA | 1.95 | 0.48 |
| 4:AB:157:THR:O | 4:AB:159:VAL:HG23 | 2.13 | 0.48 |
| 5:AC:563:GLY:HA3 | 5:AC:566:TYR:OH | 2.12 | 0.48 |
| 5:AE:188:VAL:HG23 | 5:AE:225:LEU:HD22 | 1.95 | 0.48 |
| 5:AE:39:ASP:HB2 | 5:AE:44:TYR:CE2 | 2.48 | 0.48 |
| 7:AJ:515:TRP:CD1 | 7:BA:440:GLN:HB3 | 2.48 | 0.48 |
| 7:BA:8:HIS:ND1 | 7:BA:8:HIS:O | 2.46 | 0.48 |
| 10:BE:142:ARG:O | 10:BE:143:PHE:HD1 | 1.96 | 0.48 |
| 1:BH:543:THR:OG1 | 1:BH:544:ASP:N | 2.45 | 0.48 |
| 1:BH:64:THR:HA | 1:BH:67:ILE:HG22 | 1.95 | 0.48 |
| 2:BJ:916:TYR:HB3 | 2:BJ:1004:PHE:HB3 | 1.94 | 0.48 |
| 2:C:103:PHE:CE2 | 2:C:627:GLU:HA | 2.48 | 0.48 |
| 2:C:238:TYR:HB3 | 2:C:247:VAL:HG12 | 1.94 | 0.48 |
| 2:C:357:ILE:HG12 | 2:C:358:THR:H | 1.77 | 0.48 |
| 3:CB:95:TRP:HD1 | 3:CB:106:PHE:HE2 | 1.61 | 0.48 |
| 4:CC:193:HIS:HA | 4:CC:260:TYR:HD1 | 1.77 | 0.48 |
| 4:CE:157:THR:O | 4:CE:159:VAL:HG23 | 2.13 | 0.48 |
| 5:CF:154:ILE:HG23 | 5:CG:153:LYS:HZ1 | 1.78 | 0.48 |
| 5:CH:117:ILE:HA | 5:CH:143:TRP:HB2 | 1.94 | 0.48 |
| 5:CG:316:ILE:HD13 | 6:CI:7:LYS:HE3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:31:GLY:O | 3:D:291:LYS:NZ | 2.31 | 0.48 |
| 7:DB:61:PRO:HD3 | 7:DB:74:LYS:HB3 | 1.94 | 0.48 |
| 7:DB:191:VAL:C | 7:DC:188:GLN:HA | 2.33 | 0.48 |
| 7:DC:180:GLU:HG2 | 7:DD:179:SER:OG | 2.13 | 0.48 |
| 7:DD:8:HIS:O | 7:DD:8:HIS:ND1 | 2.46 | 0.48 |
| 10:DH:142:ARG:O | 10:DH:143:PHE:HD1 | 1.96 | 0.48 |
| 11:DI:124:ILE:HG22 | 11:DI:135:ASP:O | 2.13 | 0.48 |
| 1:EA:378:PRO:HG3 | 1:EA:384:LEU:HG | 1.94 | 0.48 |
| 1:EA:543:THR:OG1 | 1:EA:544:ASP:N | 2.45 | 0.48 |
| 1:EA:636:ASP:N | 1:EA:636:ASP:OD1 | 2.44 | 0.48 |
| 2:EC:314:THR:CG2 | 2:EC:317:TYR:HB2 | 2.43 | 0.48 |
| 3:ED:43:ARG:N | 3:ED:74:HIS:HB3 | 2.28 | 0.48 |
| 4:EH:139:VAL:HG21 | 4:EH:146:VAL:HG21 | 1.94 | 0.48 |
| 5:EI:275:SER:OG | 5:EI:282:VAL:HG12 | 2.13 | 0.48 |
| 5:EJ:115:ASP:HB3 | 5:EJ:141:GLY:O | 2.13 | 0.48 |
| 6:FB:218:THR:HB | 7:HI:205:ARG:NH1 | 2.25 | 0.48 |
| 5:EJ:316:ILE:HD13 | 6:FB:7:LYS:HE3 | 1.95 | 0.48 |
| 7:FE:493:GLU:HA | 7:FE:496:ARG:NH2 | 2.28 | 0.48 |
| 7:FE:61:PRO:HD3 | 7:FE:74:LYS:HB3 | 1.94 | 0.48 |
| 7:FF:118:PRO:HG3 | 7:FG:106:ALA:HA | 1.95 | 0.48 |
| 7:FG:196:VAL:HA | 7:FG:199:VAL:HG22 | 1.95 | 0.48 |
| 7:FG:26:PRO:HA | 7:FG:27:PRO:HD3 | 1.69 | 0.48 |
| 7:FG:375:TYR:HE2 | 7:FG:390:PRO:HB2 | 1.77 | 0.48 |
| 7:FG:386:ASN:HB2 | 7:FG:387:PRO:HD2 | 1.94 | 0.48 |
| 7:FG:63:GLU:OE1 | 7:FG:80:THR:HA | 2.13 | 0.48 |
| 8:FI:121:LYS:HZ2 | 8:FI:122:THR:HG1 | 1.60 | 0.48 |
| 2:EC:654:PRO:HG3 | 9:FJ:47:ARG:CD | 2.42 | 0.48 |
| 4:G:157:THR:O | 4:G:159:VAL:HG23 | 2.13 | 0.48 |
| 10:DH:143:PHE:CE2 | 10:GA:349:ARG:HD3 | 2.47 | 0.48 |
| 11:GB:124:ILE:HG22 | 11:GB:135:ASP:O | 2.13 | 0.48 |
| 1:GD:339:CYS:HA | 1:GD:344:ASP:OD2 | 2.13 | 0.48 |
| 1:GD:424:TYR:OH | 1:GD:657:PRO:HG3 | 2.13 | 0.48 |
| 1:GD:64:THR:HA | 1:GD:67:ILE:HG22 | 1.94 | 0.48 |
| 1:GE:370:GLY:C | 1:GE:404:ILE:HG13 | 2.33 | 0.48 |
| 1:GE:522:LYS:HD2 | 1:GE:530:LEU:HD13 | 1.95 | 0.48 |
| 2:GF:120:ASN:CB | 2:GF:155:PRO:HB3 | 2.35 | 0.48 |
| 2:GF:20:GLN:HG2 | 2:GF:70:ASP:CG | 2.33 | 0.48 |
| 2:GF:238:TYR:HB3 | 2:GF:247:VAL:HG12 | 1.94 | 0.48 |
| 2:GF:253:ILE:HG13 | 2:GF:300:LEU:HD21 | 1.94 | 0.48 |
| 2:GF:248:LEU:HG | 2:GF:311:ILE:CG1 | 2.43 | 0.48 |
| 4:GI:111:ASN:HD21 | 4:GI:115:SER:N | 2.10 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:30:LYS:O | 4:H:34:ASP:N | 2.45 | 0.48 |
| 5:HB:96:ARG:HD3 | 5:HB:151:ILE:HD11 | 1.94 | 0.48 |
| 5:HC:102:TRP:HB2 | 5:HC:129:ARG:O | 2.13 | 0.48 |
| 5:HC:10:VAL:HG13 | 5:HC:13:ASP:HB2 | 1.95 | 0.48 |
| 5:HC:419:ASP:OD1 | 5:HC:420:VAL:N | 2.45 | 0.48 |
| 5:HC:64:TRP:O | 5:HC:93:ILE:HG22 | 2.13 | 0.48 |
| 5:HD:148:ASN:OD1 | 5:HD:149:LYS:N | 2.46 | 0.48 |
| 5:HD:188:VAL:HG23 | 5:HD:225:LEU:HD22 | 1.95 | 0.48 |
| 5:HD:320:LEU:HB3 | 5:HD:358:VAL:HB | 1.95 | 0.48 |
| 5:HC:460:TYR:CE1 | 5:HD:458:THR:HG23 | 2.48 | 0.48 |
| 6:HE:30:MET:O | 6:HE:32:ARG:HG2 | 2.13 | 0.48 |
| 5:I:200:LEU:HD11 | 5:J:241:THR:HG21 | 1.94 | 0.48 |
| 11:IE:175:SER:HA | 14:YD:217[F]:SER:HB2 | 1.94 | 0.48 |
| 11:IE:61:ASN:O | 11:IE:65:GLY:N | 2.38 | 0.48 |
| 5:J:319:GLU:HG3 | 5:K:262:GLN:OE1 | 2.13 | 0.48 |
| 5:J:419:ASP:OD1 | 5:J:420:VAL:N | 2.45 | 0.48 |
| 5:K:206:PHE:CG | 5:K:223:VAL:HA | 2.47 | 0.48 |
| 5:K:188:VAL:HG23 | 5:K:225:LEU:HD22 | 1.95 | 0.48 |
| 5:K:313:PHE:CE1 | 6:M:8:ALA:HB1 | 2.47 | 0.48 |
| 7:O:260:ARG:HA | 7:Q:263:VAL:O | 2.12 | 0.48 |
| 7:O:399:PHE:HD2 | 7:Q:514:PRO:HG2 | 1.78 | 0.48 |
| 7:P:511:GLU:HB3 | 7:P:513:ARG:HH11 | 1.78 | 0.48 |
| 7:Q:196:VAL:HA | 7:Q:199:VAL:HG22 | 1.95 | 0.48 |
| 8:R:77:GLU:OE2 | 8:IA:117:ALA:HA | 2.12 | 0.48 |
| 10:U:222:ILE:O | 10:U:225:ILE:HG22 | 2.12 | 0.48 |
| 12:W:178:VAL:O | 12:W:181:VAL:HG12 | 2.13 | 0.48 |
| 1:Y:106:ALA:HB2 | 1:Y:280:ALA:HB1 | 1.93 | 0.48 |
| 1:Y:340:VAL:HG22 | 1:Y:341:THR:H | 1.77 | 0.48 |
| 1:Y:444:ILE:O | 1:Y:447:TYR:N | 2.45 | 0.48 |
| 13:YA:131[D]:VAL:O | 13:YA:134[D]:GLN:N | 2.46 | 0.48 |
| 13:YA:367[C]:PRO:HA | 13:YC:315[C]:LEU:HD23 | 1.94 | 0.48 |
| 13:YA:473[D]:GLN:HA | 13:YC:481[D]:PHE:O | 2.12 | 0.48 |
| 13:YA:473[E]:GLN:HA | 13:YC:481[E]:PHE:O | 2.12 | 0.48 |
| 13:YA:70[B]:GLY:O | 13:YB:393[B]:MET:HA | 2.13 | 0.48 |
| 13:YB:16[B]:GLU:CD | 13:YB:30[B]:ARG:HH11 | 2.16 | 0.48 |
| 13:YB:436[E]:ASP:OD2 | 13:YB:437[E]:ASN:N | 2.45 | 0.48 |
| 13:YB:44[B]:VAL:HG11 | 14:YD:272[B]:GLU:HB3 | 1.95 | 0.48 |
| 13:YB:554[A]:MET:N | 13:YB:554[A]:MET:SD | 2.86 | 0.48 |
| 13:YB:554[B]:MET:N | 13:YB:554[B]:MET:SD | 2.86 | 0.48 |
| 13:YB:61[B]:ILE:CG2 | 13:YC:59[B]:GLN:HA | 2.42 | 0.48 |
| 13:YB:70[E]:GLY:O | 13:YC:394[E]:GLU:N | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:109[A]:ASN:HB3 | 13:YC:112[A]:GLU:HB2 | 1.94 | 0.48 |
| 13:YC:179[F]:MET:SD | 13:YC:279[F]:ASN:ND2 | 2.76 | 0.48 |
| 13:YB:485[E]:ASP:O | 13:YC:478[E]:ASN:N | 2.45 | 0.48 |
| 13:YA:564[B]:GLN:HE22 | 13:YC:571[B]:ARG:HD3 | 1.78 | 0.48 |
| 13:YA:394[E]:GLU:N | 13:YC:70[E]:GLY:O | 2.46 | 0.48 |
| 13:YA:34[F]:LEU:HD13 | 14:YD:163[F]:THR:HG21 | 1.95 | 0.48 |
| 14:YD:16[A]:LEU:HB2 | 14:YD:70[A]:ILE:HD13 | 1.95 | 0.48 |
| 14:YD:301[C]:MET:HA | 14:YD:304[C]:TYR:CD2 | 2.47 | 0.48 |
| 14:YD:304[C]:TYR:HB3 | 14:YD:358[C]:PHE:HD1 | 1.78 | 0.48 |
| 13:YC:12[D]:VAL:HG21 | 14:YE:256[D]:HIS:CE1 | 2.48 | 0.48 |
| 14:YE:360[B]:ASN:ND2 | 14:YE:360[B]:ASN:H | 2.04 | 0.48 |
| 14:YE:16[B]:LEU:HB2 | 14:YE:70[B]:ILE:HD13 | 1.94 | 0.48 |
| 14:YE:72[B]:ILE:O | 14:YE:86[B]:ARG:N | 2.46 | 0.48 |
| 14:YF:278[D]:SER:O | 14:YF:279[D]:ARG:NH1 | 2.44 | 0.48 |
| 14:YF:301[B]:MET:HA | 14:YF:304[B]:TYR:CD2 | 2.47 | 0.48 |
| 14:YF:304[C]:TYR:HB3 | 14:YF:358[C]:PHE:HD1 | 1.78 | 0.48 |
| 14:YD:61[B]:HIS:NE2 | 14:YF:332[B]:GLN:HB3 | 2.29 | 0.48 |
| 14:YF:304[D]:TYR:HB3 | 14:YF:358[D]:PHE:HD1 | 1.78 | 0.48 |
| 14:YF:184[A]:LYS:HE3 | 14:YF:367[A]:ILE:CG2 | 2.42 | 0.48 |
| 14:YE:332[C]:GLN:HB3 | 14:YF:61[C]:HIS:NE2 | 2.28 | 0.48 |
| 2:Z:324:ASP:HB3 | 2:Z:362:LYS:HG2 | 1.95 | 0.48 |
| 2:Z:726:PHE:O | 2:Z:729:SER:OG | 2.16 | 0.48 |
| 2:Z:909:THR:HG23 | 2:Z:910:GLU:H | 1.77 | 0.48 |
| 15:ZA:29[E]:VAL:HG21 | 15:ZA:69[E]:VAL:HG13 | 1.94 | 0.48 |
| 1:A:210:THR:HG22 | 1:A:226:MET:H | 1.79 | 0.48 |
| 1:A:287:SER:HB2 | 14:YD:373[A]:LYS:HD2 | 1.95 | 0.48 |
| 1:A:339:CYS:HA | 1:A:344:ASP:OD2 | 2.13 | 0.48 |
| 4:AB:111:ASN:HD21 | 4:AB:115:SER:N | 2.10 | 0.48 |
| 4:AB:70:HIS:HB2 | 4:AB:75:TYR:CE2 | 2.47 | 0.48 |
| 5:AC:290:SER:CB | 5:AC:371:PHE:H | 2.26 | 0.48 |
| 5:AD:204:ASP:OD1 | 5:AD:205:VAL:N | 2.41 | 0.48 |
| 5:AD:64:TRP:O | 5:AD:93:ILE:HG22 | 2.13 | 0.48 |
| 5:AE:320:LEU:HB3 | 5:AE:358:VAL:HB | 1.95 | 0.48 |
| 5:AE:558:ASP:N | 5:AE:558:ASP:OD1 | 2.45 | 0.48 |
| 6:AF:40:ILE:HG13 | 6:AG:168:LEU:HD21 | 1.95 | 0.48 |
| 6:AG:30:MET:O | 6:AG:32:ARG:HG2 | 2.13 | 0.48 |
| 7:AJ:180:GLU:HG2 | 7:BA:179:SER:OG | 2.13 | 0.48 |
| 1:B:55:VAL:HG21 | 2:C:657:TYR:CE1 | 2.48 | 0.48 |
| 7:AI:173:ILE:HD11 | 7:BA:174:ALA:HB2 | 1.96 | 0.48 |
| 7:BA:266:THR:HG22 | 7:BA:280:ALA:O | 2.13 | 0.48 |
| 7:BA:338:ASP:HB2 | 7:BA:527:GLU:OE2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:BE:208:THR:HA | 10:BE:345:GLU:HG2 | 1.94 | 0.48 |
| 1:BH:63:ASN:O | 1:BH:66:TYR:N | 2.46 | 0.48 |
| 1:BI:526:PRO:HB2 | 1:BI:528:THR:HG23 | 1.94 | 0.48 |
| 2:BJ:186:ASP:HB3 | 2:BJ:189:ARG:NE | 2.28 | 0.48 |
| 2:BJ:50:PRO:O | 2:BJ:54:TYR:HB3 | 2.14 | 0.48 |
| 2:BJ:562:ASP:O | 2:BJ:565:ASP:N | 2.44 | 0.48 |
| 2:BJ:909:THR:HG23 | 2:BJ:910:GLU:H | 1.77 | 0.48 |
| 2:C:360:ASN:O | 2:C:362:LYS:HG3 | 2.13 | 0.48 |
| 2:C:909:THR:HG23 | 2:C:910:GLU:H | 1.78 | 0.48 |
| 3:CB:69:THR:O | 3:CB:73:THR:N | 2.45 | 0.48 |
| 5:CF:291:ILE:HG22 | 5:CF:292:PRO:O | 2.13 | 0.48 |
| 5:CF:52:TYR:CZ | 5:CF:60:LEU:HB3 | 2.48 | 0.48 |
| 5:CG:312:ARG:HD3 | 5:CG:317:LEU:HD12 | 1.93 | 0.48 |
| 7:DC:120:LYS:O | 7:DC:124:ALA:N | 2.46 | 0.48 |
| 7:DC:368:SER:HG | 7:DC:370:SER:HG | 1.61 | 0.48 |
| 7:DB:509:GLY:HA3 | 7:DC:441:GLN:NE2 | 2.27 | 0.48 |
| 7:DB:202:GLY:HA3 | 7:DD:216:MET:SD | 2.53 | 0.48 |
| 12:DJ:222:SER:HB3 | 12:DJ:242:THR:OG1 | 2.14 | 0.48 |
| 1:EB:41:ASN:OD1 | 1:EB:42:GLU:N | 2.37 | 0.48 |
| 2:EC:18:ALA:HA | 2:EC:102:THR:HB | 1.94 | 0.48 |
| 2:EC:774:SER:HB2 | 2:EC:836:GLY:HA3 | 1.95 | 0.48 |
| 3:ED:289:ASN:HD21 | 3:EE:233:GLN:HB2 | 1.78 | 0.48 |
| 4:EF:157:THR:O | 4:EF:159:VAL:HG23 | 2.13 | 0.48 |
| 4:EF:70:HIS:HB2 | 4:EF:75:TYR:CE2 | 2.47 | 0.48 |
| 4:EF:39:TYR:CG | 4:EG:7:LYS:HD3 | 2.47 | 0.48 |
| 5:EI:249:ASP:OD1 | 5:EJ:160:SER:HB2 | 2.13 | 0.48 |
| 5:EI:52:TYR:CZ | 5:EI:60:LEU:HB3 | 2.48 | 0.48 |
| 5:EI:97:ASP:HB3 | 5:EI:99:PHE:O | 2.13 | 0.48 |
| 5:EJ:192:ARG:HB2 | 5:EJ:245:GLU:HB2 | 1.95 | 0.48 |
| 4:F:172:GLU:OE1 | 4:G:164:ILE:HG23 | 2.13 | 0.48 |
| 6:FC:43:LEU:HD11 | 6:FD:141:THR:HG22 | 1.94 | 0.48 |
| 7:FE:163:LEU:O | 7:FE:167:GLN:N | 2.25 | 0.48 |
| 7:FG:110:VAL:HG12 | 7:FG:111:ASN:N | 2.28 | 0.48 |
| 4:G:194:ARG:HE | 4:G:259:ASN:HA | 1.78 | 0.48 |
| 4:G:193:HIS:HA | 4:G:260:TYR:HD1 | 1.77 | 0.48 |
| 1:GD:63:ASN:O | 1:GD:66:TYR:N | 2.46 | 0.48 |
| 2:GF:250:TYR:CZ | 2:GF:306:ARG:HD3 | 2.48 | 0.48 |
| 2:GF:360:ASN:O | 2:GF:362:LYS:HG3 | 2.13 | 0.48 |
| 2:GF:909:THR:HG23 | 2:GF:910:GLU:H | 1.77 | 0.48 |
| 3:GG:46:PRO:HB3 | 3:GG:51:GLU:OE2 | 2.13 | 0.48 |
| 2:GF:898:MET:HE1 | 3:GH:315:ARG:HH12 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:157:THR:O | 4:H:159:VAL:HG23 | 2.13 | 0.48 |
| 5:HB:407:TYR:CD2 | 5:HC:407:TYR:CD2 | 3.01 | 0.48 |
| 5:HB:89:TYR:O | 5:HB:91:LYS:HG2 | 2.13 | 0.48 |
| 6:HF:70:ILE:HD11 | 6:HG:74:LYS:HG3 | 1.95 | 0.48 |
| 7:HH:480:ARG:HD3 | 7:HI:462:ASN:ND2 | 2.27 | 0.48 |
| 7:HI:120:LYS:O | 7:HI:124:ALA:N | 2.46 | 0.48 |
| 7:HI:43:GLY:O | 7:HJ:42:ALA:HB3 | 2.13 | 0.48 |
| 7:HI:511:GLU:HB3 | 7:HI:513:ARG:HH11 | 1.78 | 0.48 |
| 7:HI:54:THR:HG22 | 7:HI:55:LYS:O | 2.13 | 0.48 |
| 7:HJ:171:LYS:O | 7:HJ:175:GLN:HG3 | 2.13 | 0.48 |
| 8:IA:3:VAL:HG21 | 8:IB:56:ARG:NH2 | 2.28 | 0.48 |
| 12:GC:153:ARG:NH1 | 12:IF:184:PRO:HA | 2.27 | 0.48 |
| 5:K:148:ASN:OD1 | 5:K:149:LYS:N | 2.46 | 0.48 |
| 6:L:30:MET:O | 6:L:32:ARG:HG2 | 2.13 | 0.48 |
| 7:O:134:SER:HB3 | 7:O:140:GLY:N | 2.28 | 0.48 |
| 7:Q:134:SER:H | 7:Q:142:ILE:HD11 | 1.78 | 0.48 |
| 7:Q:171:LYS:O | 7:Q:175:GLN:HG3 | 2.13 | 0.48 |
| 7:Q:63:GLU:OE1 | 7:Q:80:THR:HA | 2.13 | 0.48 |
| 1:X:344:ASP:O | 1:X:347:THR:N | 2.44 | 0.48 |
| 1:X:521:ARG:NH1 | 1:X:560:SER:O | 2.47 | 0.48 |
| 1:Y:229:THR:OG1 | 1:Y:231:ASP:OD1 | 2.31 | 0.48 |
| 1:Y:522:LYS:HD2 | 1:Y:530:LEU:HD13 | 1.95 | 0.48 |
| 1:Y:627:PRO:HG3 | 1:Y:632:ILE:HD11 | 1.94 | 0.48 |
| 13:YA:307[B]:ALA:HB1 | 13:YA:331[B]:ILE:HD11 | 1.95 | 0.48 |
| 13:YA:387[E]:TYR:CE1 | 13:YA:388[E]:PRO:HB3 | 2.48 | 0.48 |
| 13:YA:564[E]:GLN:HE22 | 13:YC:571[E]:ARG:HD3 | 1.78 | 0.48 |
| 13:YA:67[E]:SER:HB3 | 13:YB:123[E]:ARG:HB2 | 1.95 | 0.48 |
| 13:YB:460[B]:GLY:HA3 | 13:YC:453[B]:ASP:HA | 1.94 | 0.48 |
| 13:YB:474[F]:ILE:HD13 | 13:YC:470[F]:ARG:HB2 | 1.95 | 0.48 |
| 13:YB:554[E]:MET:N | 13:YB:554[E]:MET:SD | 2.86 | 0.48 |
| 13:YC:131[F]:VAL:O | 13:YC:134[F]:GLN:N | 2.47 | 0.48 |
| 13:YC:266[B]:TRP:O | 13:YC:274[B]:GLN:NE2 | 2.46 | 0.48 |
| 13:YC:16[A]:GLU:CD | 13:YC:30[A]:ARG:HH11 | 2.16 | 0.48 |
| 13:YA:367[F]:PRO:HA | 13:YC:315[F]:LEU:HD23 | 1.94 | 0.48 |
| 13:YC:307[B]:ALA:HB1 | 13:YC:331[B]:ILE:HD11 | 1.95 | 0.48 |
| 13:YC:522[D]:VAL:HG11 | 13:YC:526[D]:GLN:NE2 | 2.27 | 0.48 |
| 13:YA:546[B]:VAL:O | 13:YC:554[B]:MET:HA | 2.13 | 0.48 |
| 13:YA:557[A]:MET:HG2 | 13:YC:565[A]:TYR:CZ | 2.47 | 0.48 |
| 14:YD:45[D]:TYR:O | 14:YD:174[D]:ARG:NH2 | 2.46 | 0.48 |
| 14:YD:304[A]:TYR:HB3 | 14:YD:358[A]:PHE:HD1 | 1.78 | 0.48 |
| 14:YD:360[C]:ASN:H | 14:YD:360[C]:ASN:ND2 | 2.04 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:301[A]:MET:HA | 14:YE:304[A]:TYR:CD2 | 2.47 | 0.48 |
| 14:YE:304[A]:TYR:HB3 | 14:YE:358[A]:PHE:HD1 | 1.78 | 0.48 |
| 14:YE:184[E]:LYS:HE3 | 14:YE:367[E]:ILE:CG2 | 2.42 | 0.48 |
| 14:YE:45[D]:TYR:O | 14:YE:174[D]:ARG:NH2 | 2.46 | 0.48 |
| 14:YE:47[A]:ARG:O | 14:YE:48[A]:ASN:ND2 | 2.45 | 0.48 |
| 13:YC:34[F]:LEU:HD13 | 14:YF:163[F]:THR:HG21 | 1.94 | 0.48 |
| 14:YF:252[D]:THR:OG1 | 14:YF:271[D]:GLY:O | 2.31 | 0.48 |
| 14:YF:304[E]:TYR:HB3 | 14:YF:358[E]:PHE:HD1 | 1.78 | 0.48 |
| 14:YF:360[E]:ASN:ND2 | 14:YF:360[E]:ASN:H | 2.04 | 0.48 |
| 14:YF:360[F]:ASN:ND2 | 14:YF:360[F]:ASN:H | 2.04 | 0.48 |
| 14:YF:184[E]:LYS:HE3 | 14:YF:367[E]:ILE:CG2 | 2.42 | 0.48 |
| 15:ZA:2[B]:SER:HB3 | 15:ZA:77[B]:MET:HB3 | 1.95 | 0.48 |
| 1:A:80:MET:HE3 | 1:A:326:ARG:HA | 1.95 | 0.48 |
| 5:AC:318:GLN:HB3 | 6:AH:4:LEU:CD1 | 2.43 | 0.48 |
| 5:AC:348:THR:H | 7:DB:233:GLN:HG3 | 1.79 | 0.48 |
| 5:AD:10:VAL:HG13 | 5:AD:13:ASP:HB2 | 1.95 | 0.48 |
| 5:AD:115:ASP:HB3 | 5:AD:141:GLY:O | 2.12 | 0.48 |
| 5:AC:7:ILE:HG12 | 5:AD:24:ILE:HG13 | 1.95 | 0.48 |
| 5:AC:407:TYR:HD2 | 5:AD:407:TYR:CE2 | 2.32 | 0.48 |
| 5:AD:399:ILE:HD13 | 5:AE:399:ILE:HG22 | 1.95 | 0.48 |
| 5:AE:558:ASP:HB2 | 5:AE:559:PRO:HD2 | 1.94 | 0.48 |
| 5:AE:58:GLN:N | 5:AE:58:GLN:OE1 | 2.37 | 0.48 |
| 7:AI:451:PHE:CD1 | 7:AI:469:VAL:HG13 | 2.48 | 0.48 |
| 7:AI:97:LEU:HD23 | 7:BA:97:LEU:HD21 | 1.95 | 0.48 |
| 7:AJ:151:LEU:HD12 | 7:AJ:171:LYS:HE2 | 1.95 | 0.48 |
| 7:AJ:236:VAL:O | 7:AJ:253:ARG:NH1 | 2.46 | 0.48 |
| 1:B:185:ILE:O | 1:B:235:GLU:HG2 | 2.12 | 0.48 |
| 1:B:627:PRO:HG3 | 1:B:632:ILE:HD11 | 1.94 | 0.48 |
| 12:BG:241:VAL:HG13 | 12:BG:241:VAL:O | 2.14 | 0.48 |
| 1:BH:339:CYS:HA | 1:BH:344:ASP:OD2 | 2.12 | 0.48 |
| 1:BH:510:MET:HE3 | 1:BH:623:LEU:HD11 | 1.94 | 0.48 |
| 1:BH:377:LYS:CD | 1:BH:641:VAL:HG21 | 2.43 | 0.48 |
| 2:BJ:18:ALA:HA | 2:BJ:102:THR:HB | 1.94 | 0.48 |
| 2:C:250:TYR:CZ | 2:C:306:ARG:HD3 | 2.48 | 0.48 |
| 2:C:946:SER:OG | 2:C:947:VAL:HG13 | 2.14 | 0.48 |
| 3:CA:153:CYS:O | 3:CA:158:GLY:N | 2.42 | 0.48 |
| 3:CA:131:TYR:CD2 | 3:CA:170:PRO:HG2 | 2.47 | 0.48 |
| 3:CB:72:TRP:HZ3 | 3:CB:275:ILE:HD13 | 1.77 | 0.48 |
| 4:CC:111:ASN:HD21 | 4:CC:115:SER:N | 2.10 | 0.48 |
| 4:CE:50:VAL:C | 4:CE:52:ASN:H | 2.17 | 0.48 |
| 5:CF:318:GLN:HB3 | 6:DA:4:LEU:CD1 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:39:ASP:HB2 | 5:CH:44:TYR:CE2 | 2.48 | 0.48 |
| 5:CH:558:ASP:HB2 | 5:CH:559:PRO:HD2 | 1.94 | 0.48 |
| 7:DB:106:ALA:HB2 | 7:DB:120:LYS:HD2 | 1.94 | 0.48 |
| 7:DB:235:GLU:OE1 | 7:DB:243:VAL:HG11 | 2.12 | 0.48 |
| 7:DC:364:GLY:N | 7:DC:393:PRO:O | 2.47 | 0.48 |
| 7:DB:308:ILE:HD11 | 7:DD:306:PHE:HB3 | 1.95 | 0.48 |
| 8:DE:22:GLN:OE1 | 8:DE:116:TYR:OH | 2.25 | 0.48 |
| 11:DI:146:TYR:CE2 | 11:DI:150:LEU:HD23 | 2.48 | 0.48 |
| 3:E:40:THR:O | 3:E:273:SER:N | 2.44 | 0.48 |
| 3:E:3:ASP:OD1 | 3:E:4:SER:N | 2.45 | 0.48 |
| 2:EC:1012:LEU:HB2 | 2:EC:1027:GLN:OE1 | 2.12 | 0.48 |
| 2:EC:250:TYR:CZ | 2:EC:306:ARG:HD3 | 2.48 | 0.48 |
| 2:EC:231:TYR:CE1 | 2:EC:391:ARG:HD3 | 2.48 | 0.48 |
| 2:EC:444:SER:HB2 | 2:EC:512:PRO:HG3 | 1.94 | 0.48 |
| 1:EA:635:ARG:NH2 | 3:EE:322:MET:SD | 2.84 | 0.48 |
| 4:EG:194:ARG:HE | 4:EG:259:ASN:HA | 1.78 | 0.48 |
| 5:EI:110:VAL:HG22 | 5:EI:123:PRO:HB3 | 1.94 | 0.48 |
| 5:EI:89:TYR:O | 5:EI:91:LYS:HG2 | 2.13 | 0.48 |
| 5:EJ:166:GLU:N | 5:EJ:166:GLU:OE1 | 2.47 | 0.48 |
| 5:EJ:67:SER:CB | 5:EJ:94:ARG:HB2 | 2.44 | 0.48 |
| 5:FA:558:ASP:HB2 | 5:FA:559:PRO:HD2 | 1.94 | 0.48 |
| 7:FE:29:ILE:CG2 | 7:FE:30:THR:H | 2.18 | 0.48 |
| 8:FH:49:ILE:HD13 | 12:IF:234:ASN:OD1 | 2.14 | 0.48 |
| 10:GA:142:ARG:O | 10:GA:143:PHE:HD1 | 1.96 | 0.48 |
| 1:GD:80:MET:HE3 | 1:GD:326:ARG:HA | 1.94 | 0.48 |
| 1:GD:521:ARG:NH1 | 1:GD:560:SER:O | 2.47 | 0.48 |
| 1:GD:68:GLN:HA | 2:GF:682:GLN:NE2 | 2.28 | 0.48 |
| 1:GE:231:ASP:OD1 | 1:GE:232:GLY:N | 2.47 | 0.48 |
| 2:GF:228:ARG:HD2 | 5:HD:556:GLN:HE22 | 1.79 | 0.48 |
| 2:GF:946:SER:OG | 2:GF:947:VAL:HG13 | 2.14 | 0.48 |
| 3:GG:195:PRO:HB2 | 3:GG:197:ASP:OD1 | 2.14 | 0.48 |
| 4:GJ:85:HIS:HD2 | 4:GJ:109:PHE:HE1 | 1.62 | 0.48 |
| 5:HB:407:TYR:HD2 | 5:HC:407:TYR:CE2 | 2.31 | 0.48 |
| 5:HC:319:GLU:OE2 | 5:HC:324:VAL:HG13 | 2.13 | 0.48 |
| 5:HC:67:SER:CB | 5:HC:94:ARG:HB2 | 2.44 | 0.48 |
| 5:HD:252:SER:O | 5:HD:255:ARG:HB2 | 2.12 | 0.48 |
| 5:HD:558:ASP:HB2 | 5:HD:559:PRO:HD2 | 1.94 | 0.48 |
| 7:HH:161:THR:O | 7:HH:165:THR:HG22 | 2.13 | 0.48 |
| 7:HH:417:ASN:HB3 | 7:HH:421:GLY:HA2 | 1.94 | 0.48 |
| 7:HI:445:HIS:CE1 | 7:HJ:445:HIS:NE2 | 2.81 | 0.48 |
| 7:HJ:134:SER:H | 7:HJ:142:ILE:HD11 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HJ:85:LEU:O | 7:HJ:86:SER:OG | 2.21 | 0.48 |
| 5:I:20:ARG:HH12 | 5:I:24:ILE:HD12 | 1.78 | 0.48 |
| 5:I:496:ASP:HB3 | 5:I:500:ALA:HB2 | 1.95 | 0.48 |
| 5:I:52:TYR:CZ | 5:I:60:LEU:HB3 | 2.48 | 0.48 |
| 8:IB:10:PHE:CE2 | 8:IB:15:PHE:CE1 | 3.01 | 0.48 |
| 9:IC:18:ASP:OD1 | 9:IC:19:TRP:N | 2.46 | 0.48 |
| 5:J:115:ASP:HB3 | 5:J:141:GLY:O | 2.12 | 0.48 |
| 5:J:206:PHE:CD2 | 5:J:223:VAL:HA | 2.48 | 0.48 |
| 5:K:117:ILE:HA | 5:K:143:TRP:HB2 | 1.94 | 0.48 |
| 5:K:265:LEU:HG | 5:K:379:ASP:HB2 | 1.94 | 0.48 |
| 6:M:29:VAL:O | 6:M:32:ARG:N | 2.36 | 0.48 |
| 7:O:451:PHE:CD1 | 7:O:469:VAL:HG13 | 2.48 | 0.48 |
| 7:P:35:ALA:O | 7:P:39:ILE:HD12 | 2.13 | 0.48 |
| 7:Q:110:VAL:HG12 | 7:Q:111:ASN:N | 2.28 | 0.48 |
| 7:Q:87:TYR:HD1 | 7:Q:88:PRO:O | 1.96 | 0.48 |
| 1:X:377:LYS:CD | 1:X:641:VAL:HG21 | 2.43 | 0.48 |
| 1:X:448:TYR:HA | 1:X:452:VAL:HG12 | 1.95 | 0.48 |
| 13:YA:24[A]:LEU:HD23 | 14:YD:259[A]:LEU:CD2 | 2.43 | 0.48 |
| 13:YA:447[E]:ASN:HB3 | 13:YC:376[E]:PHE:CE2 | 2.48 | 0.48 |
| 13:YA:522[B]:VAL:HG11 | 13:YA:526[B]:GLN:NE2 | 2.27 | 0.48 |
| 13:YA:554[A]:MET:N | 13:YA:554[A]:MET:SD | 2.86 | 0.48 |
| 13:YA:554[D]:MET:SD | 13:YA:554[D]:MET:N | 2.86 | 0.48 |
| 13:YA:61[C]:ILE:HA | 13:YB:76[C]:PRO:CA | 2.43 | 0.48 |
| 13:YA:9[B]:ASN:HA | 13:YC:7[B]:ASN:ND2 | 2.17 | 0.48 |
| 13:YB:460[E]:GLY:HA3 | 13:YC:453[E]:ASP:HA | 1.94 | 0.48 |
| 13:YB:474[A]:ILE:HD13 | 13:YC:470[A]:ARG:HB2 | 1.96 | 0.48 |
| 13:YB:485[F]:ASP:O | 13:YC:478[F]:ASN:N | 2.45 | 0.48 |
| 13:YB:522[F]:VAL:HG11 | 13:YB:526[F]:GLN:NE2 | 2.27 | 0.48 |
| 13:YB:70[F]:GLY:O | 13:YC:394[F]:GLU:N | 2.45 | 0.48 |
| 13:YC:16[E]:GLU:CD | 13:YC:30[E]:ARG:HH11 | 2.16 | 0.48 |
| 13:YA:407[D]:PRO:HB3 | 13:YC:232[D]:ASN:HB3 | 1.94 | 0.48 |
| 13:YC:387[C]:TYR:CE1 | 13:YC:388[C]:PRO:HB3 | 2.49 | 0.48 |
| 13:YC:387[E]:TYR:CE1 | 13:YC:388[E]:PRO:HB3 | 2.48 | 0.48 |
| 13:YC:554[C]:MET:N | 13:YC:554[C]:MET:SD | 2.86 | 0.48 |
| 13:YC:554[E]:MET:N | 13:YC:554[E]:MET:SD | 2.86 | 0.48 |
| 13:YC:554[F]:MET:SD | 13:YC:554[F]:MET:N | 2.86 | 0.48 |
| 13:YA:565[C]:TYR:O | 13:YC:572[C]:ILE:HA | 2.14 | 0.48 |
| 14:YD:16[C]:LEU:HB2 | 14:YD:70[C]:ILE:HD13 | 1.94 | 0.48 |
| 1:BH:130:ARG:HD3 | 14:YD:181[D]:GLY:HA2 | 1.94 | 0.48 |
| 14:YD:252[A]:THR:OG1 | 14:YD:271[A]:GLY:O | 2.32 | 0.48 |
| 14:YD:184[E]:LYS:HE3 | 14:YD:367[E]:ILE:CG2 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:252[D]:THR:OG1 | 14:YE:271[D]:GLY:O | 2.31 | 0.48 |
| 14:YE:304[E]:TYR:HB3 | 14:YE:358[E]:PHE:HD1 | 1.78 | 0.48 |
| 14:YE:54[F]:PHE:CZ | 14:YE:105[F]:ILE:HD11 | 2.49 | 0.48 |
| 2:Z:1012:LEU:HB2 | 2:Z:1027:GLN:OE1 | 2.12 | 0.48 |
| 2:Z:340:PRO:O | 2:Z:342:SER:N | 2.46 | 0.48 |
| 2:Z:968:ASP:HB3 | 2:Z:972:GLU:CG | 2.42 | 0.48 |
| 15:ZA:2[E]:SER:HB3 | 15:ZA:77[E]:MET:HB3 | 1.95 | 0.48 |
| 4:AA:63:ALA:HB3 | 4:AB:83:THR:HA | 1.95 | 0.48 |
| 4:AB:193:HIS:HA | 4:AB:260:TYR:HD1 | 1.77 | 0.48 |
| 5:AC:96:ARG:HD3 | 5:AC:151:ILE:HD11 | 1.94 | 0.48 |
| 5:AC:354:THR:HG22 | 5:AC:372:ASP:CG | 2.34 | 0.48 |
| 5:AD:192:ARG:HB2 | 5:AD:245:GLU:HB2 | 1.95 | 0.48 |
| 5:AD:288:MET:CE | 5:AD:292:PRO:HD3 | 2.44 | 0.48 |
| 5:AE:501:LEU:HB3 | 5:AE:512:PRO:HB2 | 1.94 | 0.48 |
| 6:AF:10:VAL:HA | 6:AG:13:ARG:HD2 | 1.95 | 0.48 |
| 6:AG:54:SER:HA | 6:AH:164:GLN:HE22 | 1.78 | 0.48 |
| 5:AC:318:GLN:NE2 | 6:AH:7:LYS:HB3 | 2.29 | 0.48 |
| 7:AI:235:GLU:OE1 | 7:AI:243:VAL:HG11 | 2.12 | 0.48 |
| 7:AJ:120:LYS:O | 7:AJ:124:ALA:N | 2.46 | 0.48 |
| 1:B:229:THR:OG1 | 1:B:231:ASP:OD1 | 2.31 | 0.48 |
| 7:AI:471:THR:HA | 7:BA:474:GLY:O | 2.13 | 0.48 |
| 12:BG:30:PRO:HG2 | 12:BG:177:TRP:NE1 | 2.27 | 0.48 |
| 1:BH:224:TYR:HA | 1:BH:238:PHE:HB3 | 1.96 | 0.48 |
| 1:BH:510:MET:HE1 | 1:BH:623:LEU:HD21 | 1.95 | 0.48 |
| 2:BJ:415:ARG:HH22 | 2:BJ:424:ARG:NH1 | 2.11 | 0.48 |
| 2:C:314:THR:CG2 | 2:C:317:TYR:HB2 | 2.43 | 0.48 |
| 4:CC:157:THR:O | 4:CC:159:VAL:HG23 | 2.13 | 0.48 |
| 4:CE:139:VAL:HG21 | 4:CE:146:VAL:HG21 | 1.94 | 0.48 |
| 5:CG:10:VAL:HG13 | 5:CG:13:ASP:HB2 | 1.95 | 0.48 |
| 5:CF:317:LEU:HD21 | 5:CG:260:ARG:NH2 | 2.29 | 0.48 |
| 5:CH:148:ASN:OD1 | 5:CH:149:LYS:N | 2.47 | 0.48 |
| 3:D:153:CYS:O | 3:D:158:GLY:N | 2.42 | 0.48 |
| 5:CF:196:ARG:HH11 | 7:DB:5:THR:HG23 | 1.77 | 0.48 |
| 7:DC:26:PRO:HA | 7:DC:27:PRO:HD3 | 1.72 | 0.48 |
| 8:DE:10:PHE:CE2 | 8:DE:15:PHE:CE1 | 3.01 | 0.48 |
| 12:DJ:31:SER:O | 12:DJ:32:THR:OG1 | 2.30 | 0.48 |
| 1:EA:63:ASN:O | 1:EA:66:TYR:N | 2.46 | 0.48 |
| 2:EC:555:ARG:HG3 | 2:EC:557:VAL:N | 2.29 | 0.48 |
| 2:EC:947:VAL:O | 3:ED:118:PRO:HD2 | 2.13 | 0.48 |
| 3:EE:3:ASP:OD1 | 3:EE:4:SER:N | 2.45 | 0.48 |
| 4:EF:111:ASN:HD21 | 4:EF:115:SER:N | 2.10 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:EG:30:LYS:O | 4:EG:34:ASP:N | 2.45 | 0.48 |
| 5:EI:291:ILE:HG22 | 5:EI:292:PRO:O | 2.13 | 0.48 |
| 5:EJ:308:SER:HG | 5:FA:258:TYR:HD2 | 1.60 | 0.48 |
| 4:F:111:ASN:HD21 | 4:F:115:SER:N | 2.10 | 0.48 |
| 5:FA:186:TYR:HE1 | 5:FA:246:THR:HA | 1.78 | 0.48 |
| 5:FA:190:ASN:HB2 | 5:FA:247:PHE:HB2 | 1.95 | 0.48 |
| 6:FB:125:PHE:O | 6:FB:129:VAL:HG23 | 2.14 | 0.48 |
| 6:FD:30:MET:O | 6:FD:32:ARG:HG2 | 2.13 | 0.48 |
| 7:FE:480:ARG:NE | 7:FF:465:ARG:HG3 | 2.27 | 0.48 |
| 7:FE:59:PHE:CZ | 7:FF:55:LYS:HG3 | 2.47 | 0.48 |
| 7:FF:364:GLY:N | 7:FF:393:PRO:O | 2.47 | 0.48 |
| 7:FF:71:ASN:CG | 7:HJ:365:GLY:HA2 | 2.33 | 0.48 |
| 4:G:85:HIS:HD2 | 4:G:109:PHE:HE1 | 1.62 | 0.48 |
| 4:G:50:VAL:C | 4:G:52:ASN:H | 2.17 | 0.48 |
| 10:GA:205:LYS:HB2 | 10:GA:311:PHE:CZ | 2.49 | 0.48 |
| 11:GB:147:GLU:OE1 | 11:GB:147:GLU:N | 2.45 | 0.48 |
| 12:DJ:211:HIS:HE1 | 12:GC:167:GLU:HA | 1.76 | 0.48 |
| 10:GA:215:SER:O | 12:GC:191:LEU:HD13 | 2.13 | 0.48 |
| 1:GD:110:ILE:CD1 | 1:GD:302:GLU:HA | 2.44 | 0.48 |
| 1:GE:185:ILE:O | 1:GE:235:GLU:HG2 | 2.12 | 0.48 |
| 2:GF:1012:LEU:HB2 | 2:GF:1027:GLN:OE1 | 2.12 | 0.48 |
| 2:GF:415:ARG:HH22 | 2:GF:424:ARG:NH1 | 2.11 | 0.48 |
| 3:E:176:ALA:HB2 | 2:GF:507:LYS:O | 2.12 | 0.48 |
| 2:GF:516:TRP:CH2 | 2:GF:521:ASN:HB2 | 2.49 | 0.48 |
| 2:GF:548:ILE:HG23 | 2:GF:552:SER:HB2 | 1.96 | 0.48 |
| 3:GH:72:TRP:HZ3 | 3:GH:275:ILE:HD13 | 1.77 | 0.48 |
| 4:GJ:111:ASN:HD21 | 4:GJ:115:SER:N | 2.10 | 0.48 |
| 4:GJ:50:VAL:C | 4:GJ:52:ASN:H | 2.17 | 0.48 |
| 5:HB:170:GLU:HA | 5:HB:238:ILE:HG13 | 1.94 | 0.48 |
| 5:HB:45:SER:HG | 5:HD:66:LYS:HA | 1.79 | 0.48 |
| 5:HC:166:GLU:OE1 | 5:HC:166:GLU:N | 2.47 | 0.48 |
| 5:HB:200:LEU:HD11 | 5:HC:241:THR:HG21 | 1.93 | 0.48 |
| 5:HD:39:ASP:HB2 | 5:HD:44:TYR:CE2 | 2.48 | 0.48 |
| 6:HF:30:MET:O | 6:HF:32:ARG:HG2 | 2.13 | 0.48 |
| 5:HB:318:GLN:HB3 | 6:HG:4:LEU:CD1 | 2.44 | 0.48 |
| 7:HH:211:SER:O | 7:HH:215:PHE:N | 2.43 | 0.48 |
| 7:HH:493:GLU:HA | 7:HH:496:ARG:NH2 | 2.29 | 0.48 |
| 7:HH:173:ILE:HD11 | 7:HJ:174:ALA:HB2 | 1.96 | 0.48 |
| 10:ID:205:LYS:HB2 | 10:ID:311:PHE:CZ | 2.49 | 0.48 |
| 5:J:10:VAL:HG13 | 5:J:13:ASP:HB2 | 1.95 | 0.48 |
| 5:J:267:ASP:OD1 | 5:J:285:LEU:HB2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:591:PRO:HA | 5:K:520:GLY:O | 2.14 | 0.48 |
| 7:O:452:GLY:HA2 | 7:Q:482:TYR:CD2 | 2.48 | 0.48 |
| 7:P:429:CYS:SG | 7:Q:515:TRP:NE1 | 2.86 | 0.48 |
| 7:O:476:ASP:N | 7:P:470:GLY:O | 2.38 | 0.48 |
| 7:P:180:GLU:HG2 | 7:Q:179:SER:OG | 2.13 | 0.48 |
| 8:S:10:PHE:CE2 | 8:S:15:PHE:CE1 | 3.01 | 0.48 |
| 11:V:124:ILE:HG22 | 11:V:135:ASP:O | 2.13 | 0.48 |
| 1:X:336:GLN:HG2 | 1:Y:336:GLN:HG2 | 1.95 | 0.48 |
| 1:Y:117:ALA:HB3 | 1:Y:294:ASN:HA | 1.95 | 0.48 |
| 1:Y:649:GLN:N | 1:Y:649:GLN:OE1 | 2.32 | 0.48 |
| 13:YA:12[D]:VAL:HG21 | 14:YF:256[D]:HIS:CE1 | 2.48 | 0.48 |
| 13:YA:12[F]:VAL:HG21 | 14:YF:256[F]:HIS:CE1 | 2.48 | 0.48 |
| 13:YA:16[B]:GLU:CD | 13:YA:30[B]:ARG:HH11 | 2.16 | 0.48 |
| 13:YA:407[F]:PRO:HB3 | 13:YC:232[F]:ASN:HB3 | 1.94 | 0.48 |
| 13:YA:554[C]:MET:N | 13:YA:554[C]:MET:SD | 2.86 | 0.48 |
| 13:YA:565[F]:TYR:O | 13:YC:572[F]:ILE:HA | 2.13 | 0.48 |
| 13:YB:16[D]:GLU:CD | 13:YB:30[D]:ARG:HH11 | 2.16 | 0.48 |
| 13:YB:16[C]:GLU:CD | 13:YB:30[C]:ARG:HH11 | 2.17 | 0.48 |
| 13:YB:387[B]:TYR:CE1 | 13:YB:388[B]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:474[F]:ILE:HG12 | 13:YB:466[F]:ASN:HB2 | 1.93 | 0.48 |
| 13:YC:109[C]:ASN:HB3 | 13:YC:112[C]:GLU:HB2 | 1.95 | 0.48 |
| 13:YB:66[A]:MET:HE2 | 13:YC:122[A]:PRO:HB3 | 1.95 | 0.48 |
| 13:YC:131[D]:VAL:O | 13:YC:134[D]:GLN:N | 2.46 | 0.48 |
| 13:YC:307[D]:ALA:HB1 | 13:YC:331[D]:ILE:HD11 | 1.95 | 0.48 |
| 13:YB:442[E]:THR:HG21 | 13:YC:438[E]:LEU:CD2 | 2.42 | 0.48 |
| 13:YB:474[B]:ILE:HD13 | 13:YC:470[B]:ARG:HB2 | 1.95 | 0.48 |
| 13:YB:546[C]:VAL:HA | 13:YC:538[C]:VAL:O | 2.14 | 0.48 |
| 13:YC:554[B]:MET:N | 13:YC:554[B]:MET:SD | 2.86 | 0.48 |
| 13:YA:564[C]:GLN:HE22 | 13:YC:571[C]:ARG:HD3 | 1.77 | 0.48 |
| 14:YD:16[F]:LEU:HB2 | 14:YD:70[F]:ILE:HD13 | 1.94 | 0.48 |
| 14:YD:61[A]:HIS:NE2 | 14:YF:332[A]:GLN:HB3 | 2.28 | 0.48 |
| 14:YD:72[A]:ILE:O | 14:YD:86[A]:ARG:N | 2.46 | 0.48 |
| 14:YE:252[F]:THR:OG1 | 14:YE:271[F]:GLY:O | 2.32 | 0.48 |
| 14:YF:16[B]:LEU:HB2 | 14:YF:70[B]:ILE:HD13 | 1.94 | 0.48 |
| 14:YF:47[F]:ARG:O | 14:YF:48[F]:ASN:ND2 | 2.46 | 0.48 |
| 2:Z:405:VAL:N | 2:Z:414:LYS:O | 2.41 | 0.48 |
| 2:Z:777:LEU:HD12 | 2:Z:778:THR:H | 1.79 | 0.48 |
| 1:A:231:ASP:OD1 | 1:A:233:ASN:N | 2.36 | 0.48 |
| 4:AA:85:HIS:HD2 | 4:AA:109:PHE:HE1 | 1.62 | 0.48 |
| 4:AB:50:VAL:C | 4:AB:52:ASN:H | 2.17 | 0.48 |
| 5:AC:339:GLU:HG3 | 5:AC:340:VAL:HG13 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:365:ILE:HB | 5:AC:366:PRO:HD2 | 1.96 | 0.48 |
| 5:AD:360:THR:HG22 | 5:AD:366:PRO:HG3 | 1.96 | 0.48 |
| 5:AE:358:VAL:HG23 | 5:AE:371:PHE:HD1 | 1.78 | 0.48 |
| 5:AE:496:ASP:OD2 | 5:AE:499:PHE:HB2 | 2.13 | 0.48 |
| 6:AF:127:ALA:HA | 6:AF:130:ARG:HH11 | 1.79 | 0.48 |
| 6:AF:125:PHE:O | 6:AF:129:VAL:HG23 | 2.14 | 0.48 |
| 6:AF:13:ARG:NH1 | 6:AH:47:PHE:CE1 | 2.82 | 0.48 |
| 7:AI:170:ILE:HA | 7:AI:173:ILE:HG22 | 1.95 | 0.48 |
| 7:AI:29:ILE:O | 7:AI:30:THR:OG1 | 2.23 | 0.48 |
| 7:AJ:371:ASP:OD1 | 7:AJ:526:LYS:NZ | 2.45 | 0.48 |
| 7:AJ:364:GLY:N | 7:AJ:393:PRO:O | 2.47 | 0.48 |
| 5:AE:196:ARG:HD2 | 7:AJ:5:THR:OG1 | 2.13 | 0.48 |
| 7:AJ:77:THR:HG23 | 7:AJ:79:ALA:H | 1.77 | 0.48 |
| 1:B:179:TYR:CD1 | 1:B:185:ILE:HD11 | 2.49 | 0.48 |
| 7:BA:171:LYS:O | 7:BA:175:GLN:HG3 | 2.13 | 0.48 |
| 7:BA:63:GLU:OE1 | 7:BA:80:THR:HA | 2.13 | 0.48 |
| 8:BB:10:PHE:CE2 | 8:BB:15:PHE:CE1 | 3.01 | 0.48 |
| 8:BC:85:PHE:HB3 | 8:BC:137:VAL:HG21 | 1.96 | 0.48 |
| 10:BE:215:SER:O | 12:BG:191:LEU:HD13 | 2.13 | 0.48 |
| 12:BG:222:SER:HB3 | 12:BG:242:THR:OG1 | 2.13 | 0.48 |
| 1:BH:145:PHE:HD2 | 1:BH:169:GLN:OE1 | 1.97 | 0.48 |
| 1:BH:521:ARG:NH1 | 1:BH:560:SER:O | 2.47 | 0.48 |
| 1:BI:179:TYR:CD1 | 1:BI:185:ILE:HD11 | 2.49 | 0.48 |
| 1:BI:49:GLU:HA | 1:BI:54:ASN:ND2 | 2.28 | 0.48 |
| 2:C:1025:PRO:C | 2:C:1027:GLN:H | 2.17 | 0.48 |
| 3:CB:32:PRO:O | 3:CB:34:LYS:N | 2.47 | 0.48 |
| 4:CC:70:HIS:HB2 | 4:CC:75:TYR:CE2 | 2.47 | 0.48 |
| 5:CF:117:ILE:HG22 | 5:CF:143:TRP:HE3 | 1.79 | 0.48 |
| 5:CG:319:GLU:OE2 | 5:CG:324:VAL:HG13 | 2.13 | 0.48 |
| 5:CG:36:GLU:HA | 5:CG:50:LYS:HZ1 | 1.78 | 0.48 |
| 5:CG:64:TRP:O | 5:CG:93:ILE:HG22 | 2.13 | 0.48 |
| 5:CG:67:SER:CB | 5:CG:94:ARG:HB2 | 2.44 | 0.48 |
| 5:CH:289:LYS:O | 5:CH:290:SER:OG | 2.25 | 0.48 |
| 5:CH:320:LEU:HB3 | 5:CH:358:VAL:HB | 1.95 | 0.48 |
| 5:CH:501:LEU:HB3 | 5:CH:512:PRO:HB2 | 1.94 | 0.48 |
| 6:CI:125:PHE:O | 6:CI:129:VAL:HG23 | 2.14 | 0.48 |
| 3:D:289:ASN:HD21 | 3:E:233:GLN:HB2 | 1.79 | 0.48 |
| 7:DB:97:LEU:HD23 | 7:DD:97:LEU:HD21 | 1.96 | 0.48 |
| 7:DB:482:TYR:OH | 7:DC:453:GLU:HB2 | 2.14 | 0.48 |
| 11:DI:182:ASN:ND2 | 14:YD:327[D]:ASN:HD22 | 2.12 | 0.48 |
| 12:DJ:178:VAL:O | 12:DJ:181:VAL:HG12 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:282:LYS:NZ | 3:E:289:ASN:OD1 | 2.33 | 0.48 |
| 3:E:95:TRP:HD1 | 3:E:106:PHE:HE2 | 1.62 | 0.48 |
| 1:EA:110:ILE:CD1 | 1:EA:302:GLU:HA | 2.44 | 0.48 |
| 2:EC:629:GLU:OE1 | 2:EC:629:GLU:N | 2.41 | 0.48 |
| 3:ED:92:ARG:NH1 | 3:ED:94:ASP:OD2 | 2.44 | 0.48 |
| 4:EH:157:THR:O | 4:EH:159:VAL:HG23 | 2.13 | 0.48 |
| 4:EH:193:HIS:HA | 4:EH:260:TYR:HD1 | 1.77 | 0.48 |
| 5:EI:290:SER:CB | 5:EI:371:PHE:H | 2.26 | 0.48 |
| 5:EI:496:ASP:HB3 | 5:EI:500:ALA:HB2 | 1.95 | 0.48 |
| 5:EJ:352:SER:HB2 | 5:EJ:354:THR:O | 2.14 | 0.48 |
| 5:EJ:356:TYR:CE1 | 6:FB:4:LEU:HD13 | 2.48 | 0.48 |
| 5:EJ:49:TRP:HZ3 | 5:EJ:96:ARG:CD | 2.26 | 0.48 |
| 4:F:157:THR:O | 4:F:159:VAL:HG23 | 2.13 | 0.48 |
| 5:EI:164:ARG:NH1 | 5:FA:192:ARG:HD3 | 2.29 | 0.48 |
| 5:FA:188:VAL:HG23 | 5:FA:225:LEU:HD22 | 1.95 | 0.48 |
| 7:FF:35:ALA:O | 7:FF:39:ILE:HD12 | 2.13 | 0.48 |
| 7:FF:476:ASP:OD1 | 7:FF:479:ASN:ND2 | 2.40 | 0.48 |
| 1:GD:361:GLN:OE1 | 1:GD:362:THR:N | 2.42 | 0.48 |
| 1:GD:448:TYR:CE1 | 1:GD:642:PHE:HB2 | 2.49 | 0.48 |
| 1:GE:20:ILE:O | 1:GE:22:VAL:HG23 | 2.14 | 0.48 |
| 1:GE:526:PRO:HB2 | 1:GE:528:THR:HG23 | 1.94 | 0.48 |
| 2:GF:341:LEU:O | 2:GF:342:SER:HB2 | 2.13 | 0.48 |
| 2:GF:103:PHE:CE2 | 2:GF:627:GLU:HA | 2.48 | 0.48 |
| 2:GF:777:LEU:HD12 | 2:GF:778:THR:H | 1.79 | 0.48 |
| 3:GG:38:PHE:CD1 | 3:GG:80:LYS:HA | 2.49 | 0.48 |
| 3:GG:90:ILE:HD11 | 3:GG:208:ILE:HD11 | 1.96 | 0.48 |
| 3:GH:95:TRP:HD1 | 3:GH:106:PHE:HE2 | 1.61 | 0.48 |
| 4:GI:201:LYS:NZ | 4:GI:220:ASN:OD1 | 2.37 | 0.48 |
| 4:GI:7:LYS:HD3 | 4:HA:39:TYR:CG | 2.49 | 0.48 |
| 4:GI:7:LYS:HB3 | 4:HA:53:GLY:O | 2.14 | 0.48 |
| 5:HB:253:GLN:HA | 5:HB:390:LEU:HD22 | 1.96 | 0.48 |
| 5:HB:97:ASP:HB3 | 5:HB:99:PHE:O | 2.13 | 0.48 |
| 5:HC:320:LEU:HG | 5:HC:357:SER:CB | 2.42 | 0.48 |
| 5:HC:352:SER:HB2 | 5:HC:354:THR:O | 2.14 | 0.48 |
| 6:HF:73:ASN:HD21 | 6:HF:215:PHE:HE2 | 1.60 | 0.48 |
| 7:HH:176:ILE:HG23 | 7:HH:177:ALA:N | 2.28 | 0.48 |
| 7:HH:367:VAL:O | 7:HH:389:ASN:HA | 2.13 | 0.48 |
| 7:HH:471:THR:HA | 7:HJ:474:GLY:O | 2.13 | 0.48 |
| 5:I:110:VAL:HG22 | 5:I:123:PRO:HB3 | 1.94 | 0.48 |
| 5:I:194:LYS:HB3 | 5:I:196:ARG:H | 1.78 | 0.48 |
| 5:I:259:THR:OG1 | 5:I:385:TRP:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:591:PRO:HA | 5:J:520:GLY:O | 2.14 | 0.48 |
| 8:IA:10:PHE:CE2 | 8:IA:15:PHE:CE1 | 3.01 | 0.48 |
| 12:IF:222:SER:HB3 | 12:IF:242:THR:OG1 | 2.13 | 0.48 |
| 5:J:116:THR:HA | 5:J:121:ALA:HB2 | 1.96 | 0.48 |
| 5:J:316:ILE:HD13 | 6:L:7:LYS:HE3 | 1.95 | 0.48 |
| 7:O:146:SER:N | 7:P:136:GLU:OE1 | 2.46 | 0.48 |
| 7:O:417:ASN:HB3 | 7:O:421:GLY:HA2 | 1.94 | 0.48 |
| 7:P:77:THR:HG23 | 7:P:79:ALA:H | 1.77 | 0.48 |
| 7:Q:125:LEU:O | 7:Q:129:PHE:N | 2.40 | 0.48 |
| 8:R:137:VAL:HA | 8:R:155:VAL:HG12 | 1.93 | 0.48 |
| 9:T:18:ASP:OD1 | 9:T:19:TRP:N | 2.46 | 0.48 |
| 1:X:10:LEU:HD11 | 2:Z:701:TRP:HB3 | 1.96 | 0.48 |
| 1:X:145:PHE:HD2 | 1:X:169:GLN:OE1 | 1.97 | 0.48 |
| 1:X:484:MET:HG2 | 1:X:627:PRO:HD3 | 1.95 | 0.48 |
| 13:YA:131[A]:VAL:O | 13:YA:134[A]:GLN:N | 2.46 | 0.48 |
| 13:YA:387[B]:TYR:CE1 | 13:YA:388[B]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:387[A]:TYR:CE1 | 13:YA:388[A]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:546[F]:VAL:O | 13:YC:554[F]:MET:HA | 2.13 | 0.48 |
| 13:YA:554[F]:MET:SD | 13:YA:554[F]:MET:N | 2.86 | 0.48 |
| 13:YA:70[F]:GLY:O | 13:YB:393[F]:MET:HA | 2.14 | 0.48 |
| 13:YA:76[D]:PRO:C | 13:YA:98[D]:GLY:HA2 | 2.33 | 0.48 |
| 13:YA:67[A]:SER:HB3 | 13:YB:123[A]:ARG:HB2 | 1.94 | 0.48 |
| 13:YB:147[B]:ILE:O | 13:YB:151[B]:ASN:ND2 | 2.47 | 0.48 |
| 13:YB:147[C]:ILE:O | 13:YB:151[C]:ASN:ND2 | 2.47 | 0.48 |
| 13:YC:307[C]:ALA:HB1 | 13:YC:331[C]:ILE:HD11 | 1.96 | 0.48 |
| 13:YB:70[B]:GLY:O | 13:YC:394[B]:GLU:N | 2.47 | 0.48 |
| 13:YA:565[D]:TYR:O | 13:YC:572[D]:ILE:HA | 2.14 | 0.48 |
| 14:YD:16[B]:LEU:HB2 | 14:YD:70[B]:ILE:HD13 | 1.94 | 0.48 |
| 14:YD:252[F]:THR:OG1 | 14:YD:271[F]:GLY:O | 2.31 | 0.48 |
| 13:YA:24[D]:LEU:HD23 | 14:YD:259[D]:LEU:CD2 | 2.43 | 0.48 |
| 14:YD:252[C]:THR:OG1 | 14:YD:271[C]:GLY:O | 2.32 | 0.48 |
| 14:YD:310[F]:CYS:SG | 14:YD:355[F]:LEU:HB2 | 2.54 | 0.48 |
| 14:YD:47[A]:ARG:O | 14:YD:48[A]:ASN:ND2 | 2.46 | 0.48 |
| 14:YD:72[E]:ILE:O | 14:YD:86[E]:ARG:N | 2.47 | 0.48 |
| 1:EA:130:ARG:HD3 | 14:YE:181[C]:GLY:HA2 | 1.94 | 0.48 |
| 14:YE:184[B]:LYS:HE3 | 14:YE:367[B]:ILE:CG2 | 2.42 | 0.48 |
| 14:YE:252[A]:THR:OG1 | 14:YE:271[A]:GLY:O | 2.32 | 0.48 |
| 14:YE:304[F]:TYR:HB3 | 14:YE:358[F]:PHE:HD1 | 1.78 | 0.48 |
| 1:EA:287:SER:HB2 | 14:YE:373[C]:LYS:HD2 | 1.94 | 0.48 |
| 14:YE:54[B]:PHE:CZ | 14:YE:105[B]:ILE:HD11 | 2.48 | 0.48 |
| 14:YE:72[F]:ILE:O | 14:YE:86[F]:ARG:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:34[C]:LEU:HD13 | 14:YF:163[C]:THR:HG21 | 1.95 | 0.48 |
| 14:YF:252[C]:THR:OG1 | 14:YF:271[C]:GLY:O | 2.32 | 0.48 |
| 14:YF:254[F]:TYR:CD2 | 14:YF:265[F]:MET:HG2 | 2.49 | 0.48 |
| 14:YF:310[B]:CYS:SG | 14:YF:355[B]:LEU:HB2 | 2.54 | 0.48 |
| 14:YE:332[E]:GLN:HB3 | 14:YF:61[E]:HIS:NE2 | 2.27 | 0.48 |
| 2:Z:186:ASP:HB3 | 2:Z:189:ARG:NE | 2.28 | 0.48 |
| 2:Z:250:TYR:CZ | 2:Z:306:ARG:HD3 | 2.48 | 0.48 |
| 2:Z:231:TYR:CE1 | 2:Z:391:ARG:HD3 | 2.48 | 0.48 |
| 2:Z:50:PRO:O | 2:Z:54:TYR:HB3 | 2.14 | 0.48 |
| 2:Z:840:ARG:NH2 | 2:Z:843:LYS:HG2 | 2.28 | 0.48 |
| 1:A:12:ARG:O | 2:C:709:TYR:OH | 2.24 | 0.48 |
| 1:A:448:TYR:CE1 | 1:A:642:PHE:HB2 | 2.49 | 0.48 |
| 1:A:424:TYR:OH | 1:A:657:PRO:HG3 | 2.13 | 0.48 |
| 4:AA:79:VAL:N | 4:AA:97:ILE:O | 2.31 | 0.48 |
| 4:AB:22:ASP:O | 4:AB:26:ASP:N | 2.26 | 0.48 |
| 4:AB:30:LYS:O | 4:AB:34:ASP:N | 2.45 | 0.48 |
| 5:AC:170:GLU:HA | 5:AC:238:ILE:HG13 | 1.94 | 0.48 |
| 5:AC:496:ASP:HB3 | 5:AC:500:ALA:HB2 | 1.95 | 0.48 |
| 5:AD:319:GLU:OE2 | 5:AD:324:VAL:HG13 | 2.13 | 0.48 |
| 5:AE:117:ILE:HA | 5:AE:143:TRP:HB2 | 1.94 | 0.48 |
| 5:AE:148:ASN:OD1 | 5:AE:149:LYS:N | 2.46 | 0.48 |
| 5:AE:190:ASN:HB2 | 5:AE:247:PHE:HB2 | 1.95 | 0.48 |
| 5:AE:289:LYS:O | 5:AE:290:SER:OG | 2.25 | 0.48 |
| 7:AI:509:GLY:HA3 | 7:AJ:441:GLN:NE2 | 2.28 | 0.48 |
| 7:AJ:445:HIS:CE1 | 7:BA:445:HIS:NE2 | 2.81 | 0.48 |
| 11:BF:14:LYS:HE2 | 11:BF:19:ASN:HA | 1.95 | 0.48 |
| 12:BG:178:VAL:O | 12:BG:181:VAL:HG12 | 2.13 | 0.48 |
| 1:BH:110:ILE:CD1 | 1:BH:302:GLU:HA | 2.44 | 0.48 |
| 1:BI:411:PRO:HG2 | 1:BI:413:TYR:HE1 | 1.76 | 0.48 |
| 2:BJ:946:SER:OG | 2:BJ:947:VAL:HG13 | 2.14 | 0.48 |
| 2:C:1003:GLN:OE1 | 5:I:10:VAL:HA | 2.13 | 0.48 |
| 2:C:50:PRO:O | 2:C:54:TYR:HB3 | 2.14 | 0.48 |
| 2:C:774:SER:HB2 | 2:C:836:GLY:HA3 | 1.96 | 0.48 |
| 2:C:784:GLN:HG2 | 2:C:830:ARG:HG2 | 1.95 | 0.48 |
| 3:CA:195:PRO:HB2 | 3:CA:197:ASP:OD1 | 2.14 | 0.48 |
| 4:CD:85:HIS:HD2 | 4:CD:109:PHE:HE1 | 1.62 | 0.48 |
| 4:CE:201:LYS:NZ | 4:CE:220:ASN:OD1 | 2.37 | 0.48 |
| 5:CF:275:SER:OG | 5:CF:282:VAL:HG12 | 2.13 | 0.48 |
| 5:CG:49:TRP:HZ3 | 5:CG:96:ARG:CD | 2.26 | 0.48 |
| 5:CG:591:PRO:HA | 5:CH:520:GLY:O | 2.13 | 0.48 |
| 5:CF:241:THR:HG21 | 5:CH:200:LEU:CD1 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:319:GLU:HG3 | 5:CH:262:GLN:OE1 | 2.13 | 0.48 |
| 5:CG:399:ILE:HD13 | 5:CH:399:ILE:HG22 | 1.95 | 0.48 |
| 5:CH:496:ASP:OD2 | 5:CH:499:PHE:HB2 | 2.13 | 0.48 |
| 5:CG:313:PHE:HE1 | 6:CI:8:ALA:HB1 | 1.77 | 0.48 |
| 6:DA:47:PHE:CZ | 6:DA:49:GLU:HB2 | 2.49 | 0.48 |
| 7:DB:161:THR:O | 7:DB:165:THR:HG22 | 2.13 | 0.48 |
| 7:DB:95:TYR:HA | 7:DD:98:THR:O | 2.12 | 0.48 |
| 7:DC:117:THR:OG1 | 7:DD:112:ASN:HA | 2.14 | 0.48 |
| 7:DC:429:CYS:SG | 7:DD:515:TRP:NE1 | 2.86 | 0.48 |
| 7:DD:110:VAL:HG12 | 7:DD:111:ASN:N | 2.28 | 0.48 |
| 7:DB:260:ARG:HA | 7:DD:263:VAL:O | 2.13 | 0.48 |
| 7:DD:266:THR:HG22 | 7:DD:280:ALA:O | 2.13 | 0.48 |
| 11:DI:135:ASP:CG | 11:DI:136:LYS:N | 2.67 | 0.48 |
| 1:EA:361:GLN:OE1 | 1:EA:362:THR:N | 2.42 | 0.48 |
| 2:EC:229:VAL:O | 2:EC:249:GLY:HA2 | 2.14 | 0.48 |
| 2:EC:415:ARG:HH22 | 2:EC:424:ARG:NH1 | 2.11 | 0.48 |
| 2:EC:548:ILE:HG23 | 2:EC:552:SER:HB2 | 1.96 | 0.48 |
| 3:EE:32:PRO:O | 3:EE:34:LYS:N | 2.47 | 0.48 |
| 3:EE:95:TRP:HD1 | 3:EE:106:PHE:HE2 | 1.61 | 0.48 |
| 4:EG:85:HIS:HD2 | 4:EG:109:PHE:HE1 | 1.62 | 0.48 |
| 4:EG:39:TYR:CD1 | 4:EH:7:LYS:HB2 | 2.49 | 0.48 |
| 5:EI:194:LYS:O | 5:EI:242:VAL:HA | 2.13 | 0.48 |
| 5:EI:354:THR:HG22 | 5:EI:372:ASP:CG | 2.34 | 0.48 |
| 4:F:61:ILE:O | 4:G:4:GLN:NE2 | 2.42 | 0.48 |
| 5:FA:117:ILE:HA | 5:FA:143:TRP:HB2 | 1.94 | 0.48 |
| 5:FA:265:LEU:HG | 5:FA:379:ASP:HB2 | 1.94 | 0.48 |
| 5:FA:272:SER:OG | 6:FD:106:THR:N | 2.28 | 0.48 |
| 5:EI:255:ARG:NH2 | 5:FA:390:LEU:HB2 | 2.29 | 0.48 |
| 5:FA:39:ASP:HB2 | 5:FA:44:TYR:CE2 | 2.48 | 0.48 |
| 6:FB:127:ALA:HA | 6:FB:130:ARG:HH11 | 1.79 | 0.48 |
| 12:GC:222:SER:HB3 | 12:GC:242:THR:OG1 | 2.14 | 0.48 |
| 1:GD:52:ARG:HD3 | 9:IC:22:ASP:OD2 | 2.13 | 0.48 |
| 1:GD:596:ASN:OD1 | 1:GD:596:ASN:N | 2.47 | 0.48 |
| 1:GD:647:ARG:HH11 | 1:GD:650:TYR:HE2 | 1.60 | 0.48 |
| 2:GF:774:SER:HB2 | 2:GF:836:GLY:HA3 | 1.95 | 0.48 |
| 3:GH:193:GLU:HG2 | 3:GH:224:GLY:HA3 | 1.95 | 0.48 |
| 4:GI:157:THR:O | 4:GI:159:VAL:HG23 | 2.13 | 0.48 |
| 5:HB:49:TRP:HB2 | 5:HD:90:ASN:OD1 | 2.12 | 0.48 |
| 5:HD:265:LEU:HG | 5:HD:379:ASP:HB2 | 1.94 | 0.48 |
| 5:HD:430:TRP:CZ2 | 5:HD:433:VAL:HG11 | 2.49 | 0.48 |
| 5:HB:488:VAL:HG22 | 5:HD:486:VAL:HG12 | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:995:ASP:HB2 | 5:HD:7:ILE:HG22 | 1.96 | 0.48 |
| 7:HH:61:PRO:HD3 | 7:HH:74:LYS:HB3 | 1.94 | 0.48 |
| 7:HJ:196:VAL:HA | 7:HJ:199:VAL:HG22 | 1.95 | 0.48 |
| 5:I:365:ILE:HB | 5:I:366:PRO:HD2 | 1.96 | 0.48 |
| 8:IB:85:PHE:HB3 | 8:IB:137:VAL:HG21 | 1.96 | 0.48 |
| 5:J:67:SER:CB | 5:J:94:ARG:HB2 | 2.44 | 0.48 |
| 5:K:496:ASP:OD2 | 5:K:499:PHE:HB2 | 2.13 | 0.48 |
| 6:L:47:PHE:CZ | 6:L:49:GLU:HB2 | 2.49 | 0.48 |
| 6:N:47:PHE:CZ | 6:N:49:GLU:HB2 | 2.49 | 0.48 |
| 7:Q:65:GLU:O | 7:Q:69:GLY:N | 2.46 | 0.48 |
| 13:YA:131[B]:VAL:O | 13:YA:134[B]:GLN:N | 2.47 | 0.48 |
| 13:YA:131[C]:VAL:O | 13:YA:134[C]:GLN:N | 2.47 | 0.48 |
| 13:YA:394[F]:GLU:N | 13:YC:70[F]:GLY:O | 2.46 | 0.48 |
| 13:YA:565[B]:TYR:O | 13:YC:572[B]:ILE:HA | 2.14 | 0.48 |
| 13:YA:95[A]:ILE:HD11 | 13:YB:83[A]:TYR:CZ | 2.48 | 0.48 |
| 13:YB:307[D]:ALA:HB1 | 13:YB:331[D]:ILE:HD11 | 1.95 | 0.48 |
| 13:YB:554[D]:MET:SD | 13:YB:554[D]:MET:N | 2.86 | 0.48 |
| 13:YC:131[C]:VAL:O | 13:YC:134[C]:GLN:N | 2.47 | 0.48 |
| 13:YC:131[E]:VAL:O | 13:YC:134[E]:GLN:N | 2.47 | 0.48 |
| 13:YC:131[A]:VAL:O | 13:YC:134[A]:GLN:N | 2.47 | 0.48 |
| 13:YC:16[D]:GLU:CD | 13:YC:30[D]:ARG:HH11 | 2.16 | 0.48 |
| 13:YA:447[C]:ASN:HB3 | 13:YC:376[C]:PHE:CE2 | 2.49 | 0.48 |
| 13:YB:546[D]:VAL:HA | 13:YC:538[D]:VAL:O | 2.14 | 0.48 |
| 14:YD:184[F]:LYS:HE3 | 14:YD:367[F]:ILE:CG2 | 2.42 | 0.48 |
| 14:YD:254[D]:TYR:CD2 | 14:YD:265[D]:MET:HG2 | 2.49 | 0.48 |
| 14:YD:252[B]:THR:OG1 | 14:YD:271[B]:GLY:O | 2.32 | 0.48 |
| 14:YD:184[C]:LYS:HE3 | 14:YD:367[C]:ILE:CG2 | 2.42 | 0.48 |
| 14:YD:184[D]:LYS:HE3 | 14:YD:367[D]:ILE:CG2 | 2.42 | 0.48 |
| 14:YD:54[F]:PHE:CZ | 14:YD:105[F]:ILE:HD11 | 2.49 | 0.48 |
| 14:YE:16[A]:LEU:HB2 | 14:YE:70[A]:ILE:HD13 | 1.95 | 0.48 |
| 14:YE:16[F]:LEU:HB2 | 14:YE:70[F]:ILE:HD13 | 1.94 | 0.48 |
| 14:YE:254[F]:TYR:CD2 | 14:YE:265[F]:MET:HG2 | 2.49 | 0.48 |
| 14:YE:360[A]:ASN:ND2 | 14:YE:360[A]:ASN:H | 2.04 | 0.48 |
| 14:YE:54[A]:PHE:CZ | 14:YE:105[A]:ILE:HD11 | 2.48 | 0.48 |
| 14:YE:72[C]:ILE:O | 14:YE:86[C]:ARG:N | 2.47 | 0.48 |
| 14:YF:254[D]:TYR:CD2 | 14:YF:265[D]:MET:HG2 | 2.49 | 0.48 |
| 14:YF:278[C]:SER:O | 14:YF:279[C]:ARG:NH1 | 2.44 | 0.48 |
| 14:YF:310[A]:CYS:SG | 14:YF:355[A]:LEU:HB2 | 2.54 | 0.48 |
| 14:YF:184[B]:LYS:HE3 | 14:YF:367[B]:ILE:CG2 | 2.42 | 0.48 |
| 14:YE:332[A]:GLN:NE2 | 14:YF:97[A]:VAL:HG21 | 2.29 | 0.48 |
| 14:YE:332[F]:GLN:NE2 | 14:YF:97[F]:VAL:HG21 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:430:TRP:CZ2 | 5:AE:433:VAL:HG11 | 2.49 | 0.48 |
| 1:B:117:ALA:HB3 | 1:B:294:ASN:HA | 1.95 | 0.48 |
| 7:BA:65:GLU:O | 7:BA:69:GLY:N | 2.46 | 0.48 |
| 8:BB:85:PHE:HB3 | 8:BB:137:VAL:HG21 | 1.96 | 0.48 |
| 10:BE:289:ASN:HB2 | 10:BE:290:PRO:HD2 | 1.95 | 0.48 |
| 1:BH:67:ILE:HD11 | 1:BI:67:ILE:HG21 | 1.96 | 0.48 |
| 2:BJ:644:ASP:O | 11:DI:84:TYR:OH | 2.29 | 0.48 |
| 2:BJ:968:ASP:HB3 | 2:BJ:972:GLU:CG | 2.42 | 0.48 |
| 2:C:248:LEU:HG | 2:C:311:ILE:CG1 | 2.43 | 0.48 |
| 2:C:516:TRP:CH2 | 2:C:521:ASN:HB2 | 2.49 | 0.48 |
| 1:A:10:LEU:HD11 | 2:C:701:TRP:HB3 | 1.96 | 0.48 |
| 4:CC:85:HIS:HD2 | 4:CC:109:PHE:HE1 | 1.62 | 0.48 |
| 4:CE:193:HIS:HA | 4:CE:260:TYR:HD1 | 1.77 | 0.48 |
| 5:CF:182:ARG:NH2 | 5:CG:299:ILE:HG21 | 2.28 | 0.48 |
| 5:CF:258:TYR:OH | 5:CF:260:ARG:HB2 | 2.14 | 0.48 |
| 5:CG:166:GLU:N | 5:CG:166:GLU:OE1 | 2.47 | 0.48 |
| 5:CG:352:SER:HB2 | 5:CG:354:THR:O | 2.14 | 0.48 |
| 5:CG:357:SER:OG | 6:CI:4:LEU:HD21 | 2.14 | 0.48 |
| 6:CJ:70:ILE:HD11 | 6:DA:74:LYS:HG3 | 1.95 | 0.48 |
| 3:D:46:PRO:HB3 | 3:D:51:GLU:OE2 | 2.13 | 0.48 |
| 7:DB:170:ILE:HA | 7:DB:173:ILE:HG22 | 1.95 | 0.48 |
| 7:DC:371:ASP:OD1 | 7:DC:526:LYS:NZ | 2.45 | 0.48 |
| 7:DC:511:GLU:CD | 7:DC:513:ARG:HD3 | 2.34 | 0.48 |
| 6:AF:184:SER:HA | 7:DD:149:GLN:OE1 | 2.14 | 0.48 |
| 5:CG:240:ASP:OD1 | 7:DD:4:ASN:ND2 | 2.47 | 0.48 |
| 12:DJ:187:GLY:O | 12:DJ:188:LEU:HD12 | 2.14 | 0.48 |
| 12:DJ:241:VAL:HG13 | 12:DJ:241:VAL:O | 2.14 | 0.48 |
| 1:EA:224:TYR:HA | 1:EA:238:PHE:HB3 | 1.96 | 0.48 |
| 1:EA:647:ARG:HH11 | 1:EA:650:TYR:HE2 | 1.60 | 0.48 |
| 1:EA:64:THR:HA | 1:EA:67:ILE:HG22 | 1.94 | 0.48 |
| 1:EB:619:GLN:N | 1:EB:619:GLN:OE1 | 2.35 | 0.48 |
| 1:EB:649:GLN:N | 1:EB:649:GLN:OE1 | 2.32 | 0.48 |
| 2:EC:360:ASN:O | 2:EC:362:LYS:HG3 | 2.13 | 0.48 |
| 3:ED:47:TRP:HZ3 | 3:ED:270:ARG:HD3 | 1.79 | 0.48 |
| 4:EF:85:HIS:HD2 | 4:EF:109:PHE:HE1 | 1.62 | 0.48 |
| 4:EF:193:HIS:HA | 4:EF:260:TYR:HD1 | 1.77 | 0.48 |
| 4:EG:50:VAL:C | 4:EG:52:ASN:H | 2.17 | 0.48 |
| 5:EI:20:ARG:HH12 | 5:EI:24:ILE:HD12 | 1.78 | 0.48 |
| 5:EJ:103:ASN:CG | 5:EJ:104:VAL:H | 2.17 | 0.48 |
| 5:EJ:319:GLU:OE2 | 5:EJ:324:VAL:HG13 | 2.13 | 0.48 |
| 5:EJ:416:ILE:O | 5:EJ:438:SER:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:48:ALA:C | 5:EJ:49:TRP:HD1 | 2.17 | 0.48 |
| 6:FC:125:PHE:O | 6:FC:129:VAL:HG23 | 2.14 | 0.48 |
| 7:FF:120:LYS:O | 7:FF:124:ALA:N | 2.46 | 0.48 |
| 1:GE:19:GLU:O | 1:GE:19:GLU:HG2 | 2.12 | 0.48 |
| 1:GE:392:ILE:HG23 | 1:GE:408:ILE:HD13 | 1.94 | 0.48 |
| 2:GF:229:VAL:O | 2:GF:249:GLY:HA2 | 2.14 | 0.48 |
| 2:GF:555:ARG:HG3 | 2:GF:557:VAL:N | 2.29 | 0.48 |
| 4:GJ:157:THR:O | 4:GJ:159:VAL:HG23 | 2.13 | 0.48 |
| 4:H:107:VAL:O | 4:H:148:LEU:N | 2.39 | 0.48 |
| 4:HA:70:HIS:HB2 | 4:HA:75:TYR:CE2 | 2.47 | 0.48 |
| 5:HB:255:ARG:NE | 5:HD:390:LEU:HD12 | 2.27 | 0.48 |
| 5:HC:116:THR:HA | 5:HC:121:ALA:HB2 | 1.96 | 0.48 |
| 5:HB:317:LEU:HD21 | 5:HC:260:ARG:NH2 | 2.29 | 0.48 |
| 5:HD:313:PHE:CE1 | 6:HF:8:ALA:HB1 | 2.47 | 0.48 |
| 7:HI:35:ALA:O | 7:HI:39:ILE:HD12 | 2.13 | 0.48 |
| 5:I:170:GLU:HA | 5:I:238:ILE:HG13 | 1.94 | 0.48 |
| 5:I:186:TYR:HB3 | 5:I:227:GLY:O | 2.14 | 0.48 |
| 5:I:291:ILE:HG22 | 5:I:292:PRO:O | 2.13 | 0.48 |
| 5:I:96:ARG:HD3 | 5:I:151:ILE:HD11 | 1.94 | 0.48 |
| 5:J:288:MET:CE | 5:J:292:PRO:HD3 | 2.44 | 0.48 |
| 5:J:399:ILE:HD13 | 5:K:399:ILE:HG22 | 1.95 | 0.48 |
| 5:K:430:TRP:CZ2 | 5:K:433:VAL:HG11 | 2.49 | 0.48 |
| 6:M:47:PHE:CZ | 6:M:49:GLU:HB2 | 2.49 | 0.48 |
| 7:O:367:VAL:O | 7:O:389:ASN:HA | 2.13 | 0.48 |
| 7:P:117:THR:OG1 | 7:Q:112:ASN:HA | 2.14 | 0.48 |
| 7:P:119:ALA:O | 7:P:122:THR:OG1 | 2.24 | 0.48 |
| 7:P:445:HIS:CE1 | 7:Q:445:HIS:NE2 | 2.81 | 0.48 |
| 7:Q:266:THR:HG22 | 7:Q:280:ALA:O | 2.13 | 0.48 |
| 1:X:210:THR:HG22 | 1:X:225:TYR:HA | 1.95 | 0.48 |
| 1:X:596:ASN:N | 1:X:596:ASN:OD1 | 2.47 | 0.48 |
| 1:Y:179:TYR:CD1 | 1:Y:185:ILE:HD11 | 2.49 | 0.48 |
| 1:Y:518:ASN:OD1 | 1:Y:535:LEU:HB3 | 2.12 | 0.48 |
| 13:YA:131[E]:VAL:O | 13:YA:134[E]:GLN:N | 2.47 | 0.48 |
| 13:YA:16[D]:GLU:CD | 13:YA:30[D]:ARG:HH11 | 2.16 | 0.48 |
| 13:YA:179[D]:MET:SD | 13:YA:279[D]:ASN:ND2 | 2.76 | 0.48 |
| 13:YA:307[F]:ALA:HB1 | 13:YA:331[F]:ILE:HD11 | 1.96 | 0.48 |
| 13:YA:387[D]:TYR:CE1 | 13:YA:388[D]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:387[C]:TYR:CE1 | 13:YA:388[C]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:564[F]:GLN:HE22 | 13:YC:571[F]:ARG:HD3 | 1.77 | 0.48 |
| 13:YB:16[F]:GLU:CD | 13:YB:30[F]:ARG:HH11 | 2.17 | 0.48 |
| 13:YB:460[C]:GLY:HA3 | 13:YC:453[C]:ASP:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:554[F]:MET:N | 13:YB:554[F]:MET:SD | 2.86 | 0.48 |
| 13:YA:7[A]:ASN:ND2 | 13:YB:9[A]:ASN:HA | 2.22 | 0.48 |
| 13:YA:7[C]:ASN:ND2 | 13:YB:9[C]:ASN:HA | 2.22 | 0.48 |
| 13:YC:34[E]:LEU:HD13 | 14:YF:163[E]:THR:HG21 | 1.95 | 0.48 |
| 13:YB:158[B]:PRO:HB2 | 13:YC:473[B]:GLN:OE1 | 2.14 | 0.48 |
| 13:YC:76[B]:PRO:HB2 | 13:YC:98[B]:GLY:N | 2.29 | 0.48 |
| 14:YD:254[B]:TYR:CD2 | 14:YD:265[B]:MET:HG2 | 2.49 | 0.48 |
| 14:YD:252[D]:THR:OG1 | 14:YD:271[D]:GLY:O | 2.31 | 0.48 |
| 14:YD:47[B]:ARG:O | 14:YD:48[B]:ASN:ND2 | 2.45 | 0.48 |
| 14:YD:72[B]:ILE:O | 14:YD:86[B]:ARG:N | 2.46 | 0.48 |
| 14:YE:184[D]:LYS:HE3 | 14:YE:367[D]:ILE:CG2 | 2.42 | 0.48 |
| 14:YE:254[B]:TYR:CD2 | 14:YE:265[B]:MET:HG2 | 2.49 | 0.48 |
| 14:YE:304[D]:TYR:HB3 | 14:YE:358[D]:PHE:HD1 | 1.78 | 0.48 |
| 1:GD:287:SER:HB2 | 14:YE:373[D]:LYS:HD2 | 1.95 | 0.48 |
| 14:YF:184[F]:LYS:HE3 | 14:YF:367[F]:ILE:CG2 | 2.42 | 0.48 |
| 10:DH:285:LEU:HA | 14:YF:215[F]:GLU:CG | 2.43 | 0.48 |
| 1:GD:287:SER:HB2 | 14:YF:373[B]:LYS:HD2 | 1.95 | 0.48 |
| 14:YF:47[D]:ARG:O | 14:YF:48[D]:ASN:ND2 | 2.45 | 0.48 |
| 14:YF:54[C]:PHE:CZ | 14:YF:105[C]:ILE:HD11 | 2.48 | 0.48 |
| 2:Z:229:VAL:O | 2:Z:249:GLY:HA2 | 2.14 | 0.48 |
| 2:Z:234:SER:HB3 | 2:Z:367:LYS:NZ | 2.29 | 0.48 |
| 2:Z:520:SER:O | 2:Z:522:THR:HG23 | 2.14 | 0.48 |
| 2:Z:543:LYS:HE2 | 2:Z:574:LYS:O | 2.14 | 0.48 |
| 1:A:110:ILE:CD1 | 1:A:302:GLU:HA | 2.44 | 0.48 |
| 1:A:64:THR:HA | 1:A:67:ILE:HG22 | 1.95 | 0.48 |
| 4:AA:139:VAL:HG21 | 4:AA:146:VAL:HG21 | 1.94 | 0.48 |
| 4:AB:212:ARG:HG3 | 4:AB:213:LYS:HG3 | 1.96 | 0.48 |
| 5:AC:259:THR:OG1 | 5:AC:385:TRP:HB2 | 2.14 | 0.48 |
| 5:AD:103:ASN:CG | 5:AD:104:VAL:H | 2.17 | 0.48 |
| 5:AE:314:ASN:ND2 | 6:AG:8:ALA:O | 2.46 | 0.48 |
| 6:AF:47:PHE:CZ | 6:AF:49:GLU:HB2 | 2.49 | 0.48 |
| 7:AI:371:ASP:OD1 | 7:AI:526:LYS:NZ | 2.47 | 0.48 |
| 7:AI:61:PRO:HD3 | 7:AI:74:LYS:HB3 | 1.94 | 0.48 |
| 7:AJ:511:GLU:CD | 7:AJ:513:ARG:HD3 | 2.34 | 0.48 |
| 7:AJ:99:ARG:HG2 | 7:AJ:100:TYR:N | 2.29 | 0.48 |
| 1:B:514:THR:HG22 | 1:B:539:ARG:HB2 | 1.96 | 0.48 |
| 1:B:645:ASP:N | 1:B:645:ASP:OD1 | 2.46 | 0.48 |
| 7:BA:365:GLY:N | 7:BA:392:LEU:HB2 | 2.29 | 0.48 |
| 7:AI:442:MET:HA | 7:BA:512:THR:HA | 1.94 | 0.48 |
| 8:BC:10:PHE:CE2 | 8:BC:15:PHE:CE1 | 3.01 | 0.48 |
| 11:BF:135:ASP:CG | 11:BF:136:LYS:N | 2.67 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:10:LEU:HD11 | 2:BJ:701:TRP:HB3 | 1.96 | 0.48 |
| 1:BI:645:ASP:N | 1:BI:645:ASP:OD1 | 2.46 | 0.48 |
| 2:BJ:196:GLU:HG2 | 2:BJ:197:GLY:N | 2.29 | 0.48 |
| 2:BJ:248:LEU:HG | 2:BJ:311:ILE:CG1 | 2.43 | 0.48 |
| 2:BJ:234:SER:HB3 | 2:BJ:367:LYS:NZ | 2.29 | 0.48 |
| 2:BJ:494:GLU:HB2 | 2:BJ:498:TRP:HB2 | 1.96 | 0.48 |
| 2:BJ:555:ARG:HG3 | 2:BJ:557:VAL:N | 2.29 | 0.48 |
| 2:BJ:774:SER:HB2 | 2:BJ:836:GLY:HA3 | 1.95 | 0.48 |
| 2:BJ:840:ARG:NH2 | 2:BJ:843:LYS:HG2 | 2.28 | 0.48 |
| 2:C:234:SER:HB3 | 2:C:367:LYS:NZ | 2.29 | 0.48 |
| 1:A:68:GLN:HA | 2:C:682:GLN:NE2 | 2.29 | 0.48 |
| 3:CA:90:ILE:HD11 | 3:CA:208:ILE:HD11 | 1.96 | 0.48 |
| 3:CA:43:ARG:HD2 | 3:CA:74:HIS:CD2 | 2.48 | 0.48 |
| 3:CA:64:SER:HG | 3:CA:67:GLY:H | 1.60 | 0.48 |
| 3:CA:289:ASN:HD21 | 3:CB:233:GLN:HB2 | 1.79 | 0.48 |
| 4:CD:114:GLY:HA3 | 4:CD:143:TYR:CE2 | 2.49 | 0.48 |
| 5:CF:253:GLN:HA | 5:CF:390:LEU:HD22 | 1.96 | 0.48 |
| 5:CF:490:TRP:NE1 | 5:CF:515:THR:O | 2.47 | 0.48 |
| 5:CH:323:THR:CG2 | 5:CH:354:THR:HG23 | 2.43 | 0.48 |
| 5:CH:358:VAL:HA | 5:CH:371:PHE:HA | 1.96 | 0.48 |
| 6:CI:127:ALA:HA | 6:CI:130:ARG:HH11 | 1.79 | 0.48 |
| 3:D:43:ARG:HD2 | 3:D:74:HIS:CD2 | 2.48 | 0.48 |
| 3:D:90:ILE:HD11 | 3:D:208:ILE:HD11 | 1.96 | 0.48 |
| 7:DB:160:MET:HG3 | 7:DB:164:LYS:NZ | 2.29 | 0.48 |
| 7:DB:367:VAL:O | 7:DB:389:ASN:HA | 2.13 | 0.48 |
| 7:DC:99:ARG:HG2 | 7:DC:100:TYR:N | 2.29 | 0.48 |
| 7:DC:511:GLU:HB3 | 7:DC:513:ARG:HH11 | 1.79 | 0.48 |
| 7:DD:338:ASP:HB2 | 7:DD:527:GLU:OE2 | 2.12 | 0.48 |
| 7:DD:73:THR:HG23 | 7:DD:74:LYS:H | 1.78 | 0.48 |
| 8:DE:85:PHE:HB3 | 8:DE:137:VAL:HG21 | 1.96 | 0.48 |
| 8:DE:3:VAL:HG21 | 8:DF:56:ARG:NH2 | 2.29 | 0.48 |
| 3:E:32:PRO:O | 3:E:34:LYS:N | 2.47 | 0.48 |
| 1:EA:448:TYR:HA | 1:EA:452:VAL:HG12 | 1.95 | 0.48 |
| 1:EA:484:MET:HG2 | 1:EA:627:PRO:HD3 | 1.95 | 0.48 |
| 1:EA:424:TYR:OH | 1:EA:657:PRO:HG3 | 2.13 | 0.48 |
| 2:EC:234:SER:HB3 | 2:EC:367:LYS:NZ | 2.29 | 0.48 |
| 2:EC:366:TYR:HB2 | 2:EC:380:ILE:CD1 | 2.41 | 0.48 |
| 2:EC:682:GLN:O | 2:EC:685:ASN:HB3 | 2.12 | 0.48 |
| 3:ED:90:ILE:HD11 | 3:ED:208:ILE:HD11 | 1.96 | 0.48 |
| 4:F:114:GLY:HA3 | 4:F:143:TYR:CE2 | 2.49 | 0.48 |
| 4:F:161:ASN:HB3 | 4:H:168:PHE:CE1 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:194:ARG:HE | 4:F:259:ASN:HA | 1.78 | 0.48 |
| 5:FA:136:VAL:O | 5:FA:143:TRP:HA | 2.14 | 0.48 |
| 6:FD:127:ALA:HA | 6:FD:130:ARG:HH11 | 1.79 | 0.48 |
| 6:FD:47:PHE:CZ | 6:FD:49:GLU:HB2 | 2.49 | 0.48 |
| 7:FE:442:MET:HA | 7:FG:512:THR:HA | 1.96 | 0.48 |
| 7:FF:142:ILE:HG22 | 7:FF:143:LYS:O | 2.14 | 0.48 |
| 7:FF:151:LEU:HD12 | 7:FF:171:LYS:HE2 | 1.95 | 0.48 |
| 7:FF:511:GLU:CD | 7:FF:513:ARG:HD3 | 2.34 | 0.48 |
| 7:FE:60:ILE:HG22 | 7:FF:52:SER:N | 2.28 | 0.48 |
| 7:FG:8:HIS:O | 7:FG:8:HIS:ND1 | 2.46 | 0.48 |
| 2:GF:340:PRO:O | 2:GF:342:SER:N | 2.46 | 0.48 |
| 2:GF:50:PRO:O | 2:GF:54:TYR:HB3 | 2.14 | 0.48 |
| 3:GG:131:TYR:CD2 | 3:GG:170:PRO:HG2 | 2.47 | 0.48 |
| 4:GI:222:LEU:HD13 | 4:HA:216:THR:CG2 | 2.44 | 0.48 |
| 6:HE:127:ALA:HA | 6:HE:130:ARG:HH11 | 1.79 | 0.48 |
| 5:HB:340:VAL:HG21 | 6:HF:174:TYR:H | 1.79 | 0.48 |
| 7:HH:145:SER:O | 7:HH:164:LYS:HE2 | 2.11 | 0.48 |
| 7:HH:191:VAL:C | 7:HI:188:GLN:HA | 2.34 | 0.48 |
| 7:HH:308:ILE:HD11 | 7:HJ:306:PHE:HB3 | 1.94 | 0.48 |
| 7:HH:442:MET:HA | 7:HJ:512:THR:HA | 1.94 | 0.48 |
| 7:HH:146:SER:N | 7:HI:136:GLU:OE1 | 2.46 | 0.48 |
| 7:HI:142:ILE:HG22 | 7:HI:143:LYS:O | 2.14 | 0.48 |
| 7:HI:151:LEU:HD12 | 7:HI:171:LYS:HE2 | 1.95 | 0.48 |
| 7:HI:511:GLU:CD | 7:HI:513:ARG:HD3 | 2.34 | 0.48 |
| 7:HI:180:GLU:HG2 | 7:HJ:179:SER:OG | 2.13 | 0.48 |
| 5:I:490:TRP:NE1 | 5:I:515:THR:O | 2.47 | 0.48 |
| 11:IE:146:TYR:CE2 | 11:IE:150:LEU:HD23 | 2.48 | 0.48 |
| 12:IF:110:LEU:HG | 12:IF:177:TRP:HD1 | 1.79 | 0.48 |
| 5:J:168:LEU:HA | 5:J:241:THR:HG22 | 1.94 | 0.48 |
| 5:J:64:TRP:O | 5:J:93:ILE:HG22 | 2.13 | 0.48 |
| 5:K:164:ARG:HA | 5:K:181:PHE:HZ | 1.79 | 0.48 |
| 5:K:314:ASN:ND2 | 6:M:8:ALA:O | 2.47 | 0.48 |
| 5:K:358:VAL:HA | 5:K:371:PHE:HA | 1.96 | 0.48 |
| 5:K:558:ASP:OD1 | 5:K:558:ASP:N | 2.45 | 0.48 |
| 6:L:127:ALA:HA | 6:L:130:ARG:HH11 | 1.79 | 0.48 |
| 6:M:127:ALA:HA | 6:M:130:ARG:HH11 | 1.79 | 0.48 |
| 6:M:30:MET:O | 6:M:32:ARG:HG2 | 2.13 | 0.48 |
| 6:L:10:VAL:CG1 | 6:N:10:VAL:HG21 | 2.44 | 0.48 |
| 7:O:160:MET:HG3 | 7:O:164:LYS:NZ | 2.29 | 0.48 |
| 7:O:76:VAL:HG11 | 7:Q:81:LEU:HD22 | 1.94 | 0.48 |
| 12:W:222:SER:HB3 | 12:W:242:THR:OG1 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:525:ASN:HB3 | 1:X:528:THR:HG21 | 1.96 | 0.48 |
| 13:YA:24[B]:LEU:HD23 | 14:YD:259[B]:LEU:CD2 | 2.43 | 0.48 |
| 13:YA:24[C]:LEU:HD23 | 14:YD:259[C]:LEU:CD2 | 2.43 | 0.48 |
| 13:YA:379[B]:PRO:HG2 | 13:YA:429[B]:ARG:NE | 2.29 | 0.48 |
| 13:YA:453[A]:ASP:OD1 | 13:YC:321[A]:LYS:HG2 | 2.14 | 0.48 |
| 13:YA:70[E]:GLY:O | 13:YB:393[E]:MET:HA | 2.14 | 0.48 |
| 13:YB:24[F]:LEU:HA | 13:YB:24[F]:LEU:HD12 | 1.62 | 0.48 |
| 13:YB:292[B]:PHE:CD1 | 13:YC:364[B]:ALA:HB2 | 2.48 | 0.48 |
| 13:YB:379[E]:PRO:HG2 | 13:YB:429[E]:ARG:NE | 2.29 | 0.48 |
| 13:YC:12[F]:VAL:HG21 | 14:YE:256[F]:HIS:CE1 | 2.49 | 0.48 |
| 13:YC:24[B]:LEU:HD23 | 14:YF:259[B]:LEU:CD2 | 2.44 | 0.48 |
| 13:YC:387[B]:TYR:CE1 | 13:YC:388[B]:PRO:HB3 | 2.49 | 0.48 |
| 13:YA:546[A]:VAL:O | 13:YC:554[A]:MET:HA | 2.13 | 0.48 |
| 14:YD:301[E]:MET:HA | 14:YD:304[E]:TYR:CD2 | 2.47 | 0.48 |
| 14:YD:304[D]:TYR:HB3 | 14:YD:358[D]:PHE:HD1 | 1.78 | 0.48 |
| 14:YD:328[B]:ASP:OD1 | 14:YD:329[B]:SER:N | 2.47 | 0.48 |
| 14:YE:54[E]:PHE:CZ | 14:YE:105[E]:ILE:HD11 | 2.49 | 0.48 |
| 14:YE:185[F]:PHE:CD2 | 14:YE:297[F]:ARG:HA | 2.49 | 0.48 |
| 14:YE:214[B]:GLY:O | 14:YE:215[B]:GLU:HG3 | 2.14 | 0.48 |
| 14:YE:214[D]:GLY:O | 14:YE:215[D]:GLU:HG3 | 2.14 | 0.48 |
| 14:YE:254[C]:TYR:CD2 | 14:YE:265[C]:MET:HG2 | 2.49 | 0.48 |
| 14:YE:301[C]:MET:HA | 14:YE:304[C]:TYR:CD2 | 2.47 | 0.48 |
| 14:YE:310[D]:CYS:SG | 14:YE:355[D]:LEU:HB2 | 2.54 | 0.48 |
| 14:YE:328[A]:ASP:OD1 | 14:YE:329[A]:SER:N | 2.47 | 0.48 |
| 14:YE:304[B]:TYR:HB3 | 14:YE:358[B]:PHE:HD1 | 1.78 | 0.48 |
| 14:YE:184[A]:LYS:HE3 | 14:YE:367[A]:ILE:CG2 | 2.42 | 0.48 |
| 14:YF:16[E]:LEU:HB2 | 14:YF:70[E]:ILE:HD13 | 1.94 | 0.48 |
| 14:YF:304[B]:TYR:HB3 | 14:YF:358[B]:PHE:HD1 | 1.78 | 0.48 |
| 14:YF:328[B]:ASP:OD1 | 14:YF:329[B]:SER:N | 2.47 | 0.48 |
| 2:Z:189:ARG:HD3 | 2:Z:203:GLU:OE2 | 2.14 | 0.48 |
| 2:Z:248:LEU:HG | 2:Z:311:ILE:CG1 | 2.43 | 0.48 |
| 1:A:200:TYR:HB2 | 1:A:269:VAL:CG1 | 2.44 | 0.48 |
| 1:A:521:ARG:NH1 | 1:A:560:SER:O | 2.47 | 0.48 |
| 5:AC:117:ILE:HG22 | 5:AC:143:TRP:HE3 | 1.79 | 0.48 |
| 7:AI:154:ALA:HB3 | 7:BA:162:PRO:HG2 | 1.96 | 0.48 |
| 7:AI:160:MET:HG3 | 7:AI:164:LYS:NZ | 2.29 | 0.48 |
| 5:AC:196:ARG:HD3 | 7:AI:5:THR:HG23 | 1.95 | 0.48 |
| 7:AJ:35:ALA:O | 7:AJ:39:ILE:HD12 | 2.13 | 0.48 |
| 7:BA:253:ARG:O | 7:BA:262:VAL:HG22 | 2.14 | 0.48 |
| 12:BG:117:ALA:O | 12:BG:120:SER:OG | 2.24 | 0.48 |
| 1:BH:5:PRO:HG3 | 1:BH:36:TRP:CZ2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:424:TYR:OH | 1:BH:657:PRO:HG3 | 2.13 | 0.48 |
| 1:BH:645:ASP:N | 1:BH:645:ASP:OD1 | 2.45 | 0.48 |
| 1:BI:444:ILE:O | 1:BI:447:TYR:N | 2.45 | 0.48 |
| 1:BI:506:LYS:O | 1:BI:509:SER:OG | 2.19 | 0.48 |
| 2:BJ:360:ASN:O | 2:BJ:362:LYS:HG3 | 2.13 | 0.48 |
| 2:BJ:548:ILE:HG23 | 2:BJ:552:SER:HB2 | 1.96 | 0.48 |
| 2:BJ:85:ALA:HB2 | 2:BJ:91:GLN:HE22 | 1.79 | 0.48 |
| 2:C:189:ARG:HD3 | 2:C:203:GLU:OE2 | 2.14 | 0.48 |
| 2:C:548:ILE:HG23 | 2:C:552:SER:HB2 | 1.96 | 0.48 |
| 2:BJ:817:LEU:HD11 | 3:CB:252:TYR:CE2 | 2.47 | 0.48 |
| 4:CD:50:VAL:C | 4:CD:52:ASN:H | 2.17 | 0.48 |
| 4:CE:114:GLY:HA3 | 4:CE:143:TYR:CE2 | 2.49 | 0.48 |
| 5:CF:7:ILE:HG12 | 5:CG:24:ILE:HG13 | 1.96 | 0.48 |
| 5:CH:136:VAL:O | 5:CH:143:TRP:HA | 2.14 | 0.48 |
| 6:CI:30:MET:O | 6:CI:32:ARG:HG2 | 2.13 | 0.48 |
| 3:D:195:PRO:HB2 | 3:D:197:ASP:OD1 | 2.14 | 0.48 |
| 2:C:986:ARG:HH22 | 3:D:323:ASP:HB2 | 1.78 | 0.48 |
| 6:CJ:43:LEU:HD11 | 6:DA:141:THR:HG22 | 1.96 | 0.48 |
| 7:DB:323:GLY:HA2 | 7:DC:326:ILE:HG23 | 1.95 | 0.48 |
| 7:DB:399:PHE:HD2 | 7:DD:514:PRO:HG2 | 1.77 | 0.48 |
| 1:EA:377:LYS:CD | 1:EA:641:VAL:HG21 | 2.43 | 0.48 |
| 1:EA:508:ARG:HH22 | 1:EA:577:PHE:CA | 2.27 | 0.48 |
| 1:EB:522:LYS:HD2 | 1:EB:530:LEU:HD13 | 1.95 | 0.48 |
| 2:EC:516:TRP:CH2 | 2:EC:521:ASN:HB2 | 2.49 | 0.48 |
| 1:EA:68:GLN:HA | 2:EC:682:GLN:NE2 | 2.28 | 0.48 |
| 2:EC:840:ARG:NH2 | 2:EC:843:LYS:HG2 | 2.28 | 0.48 |
| 2:EC:85:ALA:HB2 | 2:EC:91:GLN:HE22 | 1.79 | 0.48 |
| 4:EF:200:ALA:HB3 | 4:EF:221:ILE:HD11 | 1.96 | 0.48 |
| 4:EH:50:VAL:C | 4:EH:52:ASN:H | 2.17 | 0.48 |
| 5:EJ:146:VAL:HG11 | 5:FA:151:ILE:O | 2.13 | 0.48 |
| 5:EJ:288:MET:CE | 5:EJ:292:PRO:HD3 | 2.44 | 0.48 |
| 5:EJ:304:ILE:HG21 | 5:EJ:309:LEU:HD12 | 1.96 | 0.48 |
| 5:FA:164:ARG:HA | 5:FA:181:PHE:HZ | 1.79 | 0.48 |
| 5:FA:170:GLU:O | 5:FA:171:VAL:HG12 | 2.13 | 0.48 |
| 7:FE:503:ASN:OD1 | 7:FG:446:LYS:N | 2.46 | 0.48 |
| 7:FF:511:GLU:HB3 | 7:FF:513:ARG:HH11 | 1.78 | 0.48 |
| 7:FG:476:ASP:O | 7:FG:479:ASN:ND2 | 2.47 | 0.48 |
| 8:FH:18:PRO:HD3 | 8:IA:151:GLN:N | 2.29 | 0.48 |
| 10:GA:289:ASN:HB2 | 10:GA:290:PRO:HD2 | 1.95 | 0.48 |
| 1:GD:112:LEU:HD13 | 1:GD:297:VAL:HG12 | 1.96 | 0.48 |
| 1:GD:145:PHE:HD2 | 1:GD:169:GLN:OE1 | 1.97 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:378:PRO:HG3 | 1:GD:384:LEU:HG | 1.94 | 0.48 |
| 2:GF:923:SER:HB3 | 2:GF:992:PRO:HG2 | 1.96 | 0.48 |
| 3:GG:225:TYR:HE2 | 3:GG:231:TRP:HB3 | 1.79 | 0.48 |
| 3:GG:43:ARG:HD2 | 3:GG:74:HIS:CD2 | 2.49 | 0.48 |
| 5:HB:186:TYR:HB3 | 5:HB:227:GLY:O | 2.14 | 0.48 |
| 5:HB:194:LYS:O | 5:HB:242:VAL:HA | 2.13 | 0.48 |
| 5:HB:52:TYR:CZ | 5:HB:60:LEU:HB3 | 2.48 | 0.48 |
| 5:HC:49:TRP:HZ3 | 5:HC:96:ARG:CD | 2.26 | 0.48 |
| 5:HC:189:ASN:HD21 | 5:HD:150:GLN:HE22 | 1.62 | 0.48 |
| 5:HD:359:GLU:O | 5:HD:370:HIS:N | 2.36 | 0.48 |
| 6:HF:43:LEU:HD11 | 6:HG:141:THR:HG22 | 1.96 | 0.48 |
| 7:HH:160:MET:HG3 | 7:HH:164:LYS:NZ | 2.29 | 0.48 |
| 7:HH:263:VAL:O | 7:HI:260:ARG:HA | 2.14 | 0.48 |
| 7:HH:477:TRP:CZ3 | 7:HI:469:VAL:HB | 2.49 | 0.48 |
| 7:HH:504:ARG:HA | 7:HJ:422:LYS:HB3 | 1.95 | 0.48 |
| 7:HI:99:ARG:HG2 | 7:HI:100:TYR:N | 2.29 | 0.48 |
| 5:HD:196:ARG:HH22 | 7:HI:9:VAL:HG13 | 1.78 | 0.48 |
| 7:HJ:110:VAL:HG12 | 7:HJ:111:ASN:N | 2.28 | 0.48 |
| 7:HJ:335:ASN:OD1 | 7:HJ:336:GLU:N | 2.47 | 0.48 |
| 5:J:147:LYS:HE2 | 5:J:155:THR:HB | 1.94 | 0.48 |
| 5:J:321:ALA:HA | 5:J:358:VAL:HB | 1.95 | 0.48 |
| 5:J:352:SER:HB2 | 5:J:354:THR:O | 2.14 | 0.48 |
| 5:J:506:LEU:HD23 | 5:J:512:PRO:HA | 1.96 | 0.48 |
| 5:J:11:VAL:HG13 | 5:K:20:ARG:HG2 | 1.94 | 0.48 |
| 7:O:161:THR:O | 7:O:165:THR:HG22 | 2.13 | 0.48 |
| 7:P:99:ARG:HG2 | 7:P:100:TYR:N | 2.29 | 0.48 |
| 7:P:511:GLU:CD | 7:P:513:ARG:HD3 | 2.34 | 0.48 |
| 7:P:118:PRO:HG3 | 7:Q:106:ALA:HA | 1.96 | 0.48 |
| 7:O:95:TYR:HA | 7:Q:98:THR:O | 2.14 | 0.48 |
| 8:R:140:LEU:HD23 | 8:IA:41:LEU:HD22 | 1.96 | 0.48 |
| 8:R:3:VAL:HG21 | 8:S:56:ARG:NH2 | 2.28 | 0.48 |
| 1:X:430:GLN:OE1 | 1:X:430:GLN:N | 2.29 | 0.48 |
| 1:X:448:TYR:CE1 | 1:X:642:PHE:HB2 | 2.49 | 0.48 |
| 13:YA:109[F]:ASN:HB3 | 13:YA:112[F]:GLU:HB2 | 1.95 | 0.48 |
| 13:YA:67[B]:SER:HB3 | 13:YB:123[B]:ARG:HB2 | 1.96 | 0.48 |
| 13:YA:70[C]:GLY:O | 13:YB:393[C]:MET:HA | 2.14 | 0.48 |
| 13:YA:76[B]:PRO:HB2 | 13:YA:98[B]:GLY:N | 2.29 | 0.48 |
| 13:YB:109[C]:ASN:HB3 | 13:YB:112[C]:GLU:HB2 | 1.94 | 0.48 |
| 13:YB:16[A]:GLU:CD | 13:YB:30[A]:ARG:HH11 | 2.16 | 0.48 |
| 13:YB:307[F]:ALA:HB1 | 13:YB:331[F]:ILE:HD11 | 1.96 | 0.48 |
| 13:YB:379[B]:PRO:HG2 | 13:YB:429[B]:ARG:NE | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:474[E]:ILE:HD13 | 13:YC:470[E]:ARG:HB2 | 1.95 | 0.48 |
| 13:YA:447[B]:ASN:HB3 | 13:YC:376[B]:PHE:CE2 | 2.48 | 0.48 |
| 13:YC:379[B]:PRO:HG2 | 13:YC:429[B]:ARG:NE | 2.29 | 0.48 |
| 13:YC:387[F]:TYR:CE1 | 13:YC:388[F]:PRO:HB3 | 2.49 | 0.48 |
| 13:YC:387[D]:TYR:CE1 | 13:YC:388[D]:PRO:HB3 | 2.49 | 0.48 |
| 13:YC:554[D]:MET:N | 13:YC:554[D]:MET:SD | 2.86 | 0.48 |
| 13:YB:571[A]:ARG:HD3 | 13:YC:564[A]:GLN:HE22 | 1.78 | 0.48 |
| 13:YB:61[F]:ILE:HG12 | 13:YC:60[F]:PRO:HD3 | 1.96 | 0.48 |
| 14:YD:252[E]:THR:OG1 | 14:YD:271[E]:GLY:O | 2.31 | 0.48 |
| 14:YD:254[E]:TYR:CD2 | 14:YD:265[E]:MET:HG2 | 2.49 | 0.48 |
| 14:YD:304[F]:TYR:HB3 | 14:YD:358[F]:PHE:HD1 | 1.78 | 0.48 |
| 14:YD:310[E]:CYS:SG | 14:YD:355[E]:LEU:HB2 | 2.54 | 0.48 |
| 14:YE:185[A]:PHE:CD2 | 14:YE:297[A]:ARG:HA | 2.49 | 0.48 |
| 14:YE:254[E]:TYR:CD2 | 14:YE:265[E]:MET:HG2 | 2.49 | 0.48 |
| 14:YE:310[C]:CYS:SG | 14:YE:355[C]:LEU:HB2 | 2.54 | 0.48 |
| 14:YE:328[F]:ASP:OD1 | 14:YE:329[F]:SER:N | 2.47 | 0.48 |
| 14:YD:95[B]:VAL:O | 14:YF:236[B]:TRP:N | 2.47 | 0.48 |
| 14:YF:252[B]:THR:OG1 | 14:YF:271[B]:GLY:O | 2.32 | 0.48 |
| 14:YF:254[C]:TYR:CD2 | 14:YF:265[C]:MET:HG2 | 2.49 | 0.48 |
| 14:YF:252[F]:THR:OG1 | 14:YF:271[F]:GLY:O | 2.32 | 0.48 |
| 14:YF:301[A]:MET:HA | 14:YF:304[A]:TYR:CD2 | 2.47 | 0.48 |
| 1:X:287:SER:HB2 | 14:YF:373[D]:LYS:HD2 | 1.96 | 0.48 |
| 2:Z:516:TRP:CH2 | 2:Z:521:ASN:HB2 | 2.49 | 0.48 |
| 2:Z:548:ILE:HG23 | 2:Z:552:SER:HB2 | 1.96 | 0.48 |
| 1:A:596:ASN:OD1 | 1:A:596:ASN:N | 2.47 | 0.48 |
| 1:A:484:MET:HG2 | 1:A:627:PRO:HD3 | 1.95 | 0.48 |
| 4:AA:114:GLY:HA3 | 4:AA:143:TYR:CE2 | 2.49 | 0.48 |
| 4:AA:50:VAL:C | 4:AA:52:ASN:H | 2.17 | 0.48 |
| 5:AC:258:TYR:OH | 5:AC:260:ARG:HB2 | 2.14 | 0.48 |
| 5:AC:490:TRP:NE1 | 5:AC:515:THR:O | 2.47 | 0.48 |
| 5:AE:139:ALA:HB3 | 5:AE:140:PRO:HD3 | 1.96 | 0.48 |
| 5:AE:396:LYS:O | 5:AE:399:ILE:HG13 | 2.14 | 0.48 |
| 6:AH:127:ALA:HA | 6:AH:130:ARG:HH11 | 1.79 | 0.48 |
| 6:AH:47:PHE:CZ | 6:AH:49:GLU:HB2 | 2.49 | 0.48 |
| 7:AI:146:SER:N | 7:AJ:136:GLU:OE1 | 2.47 | 0.48 |
| 7:AI:479:ASN:O | 7:AJ:468:PHE:HB2 | 2.13 | 0.48 |
| 7:AI:493:GLU:HA | 7:AI:496:ARG:NH2 | 2.28 | 0.48 |
| 1:B:209:TRP:HE3 | 1:B:212:LYS:CB | 2.26 | 0.48 |
| 8:BC:121:LYS:HZ2 | 8:BC:122:THR:HG1 | 1.62 | 0.48 |
| 1:BH:210:THR:HG22 | 1:BH:225:TYR:HA | 1.95 | 0.48 |
| 1:BH:508:ARG:HH22 | 1:BH:577:PHE:CA | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:179:TYR:HD1 | 1:BI:185:ILE:HD11 | 1.79 | 0.48 |
| 2:BJ:1013:LYS:HB3 | 3:CA:206:GLU:OE2 | 2.13 | 0.48 |
| 2:BJ:486:HIS:HD2 | 3:ED:65:VAL:HG13 | 1.78 | 0.48 |
| 2:BJ:853:ASP:OD1 | 2:BJ:854:TYR:N | 2.47 | 0.48 |
| 2:C:193:MET:O | 2:C:200:TYR:N | 2.36 | 0.48 |
| 2:C:454:ASN:HB2 | 2:C:471:VAL:HG21 | 1.96 | 0.48 |
| 2:C:520:SER:O | 2:C:522:THR:HG23 | 2.14 | 0.48 |
| 2:C:543:LYS:HE2 | 2:C:574:LYS:O | 2.14 | 0.48 |
| 4:CC:161:ASN:HB3 | 4:CE:168:PHE:CE1 | 2.49 | 0.48 |
| 5:CG:289:LYS:HD2 | 5:CG:372:ASP:HB3 | 1.95 | 0.48 |
| 5:CF:407:TYR:HD2 | 5:CG:407:TYR:CE2 | 2.32 | 0.48 |
| 5:CF:486:VAL:HG12 | 5:CG:488:VAL:HG22 | 1.96 | 0.48 |
| 5:CG:48:ALA:C | 5:CG:49:TRP:HD1 | 2.17 | 0.48 |
| 5:CH:190:ASN:HB2 | 5:CH:247:PHE:HB2 | 1.95 | 0.48 |
| 3:D:225:TYR:HE2 | 3:D:231:TRP:HB3 | 1.79 | 0.48 |
| 3:D:38:PHE:CD1 | 3:D:80:LYS:HA | 2.49 | 0.48 |
| 1:EA:210:THR:HG22 | 1:EA:226:MET:H | 1.79 | 0.48 |
| 1:EA:448:TYR:CE1 | 1:EA:642:PHE:HB2 | 2.49 | 0.48 |
| 1:EB:179:TYR:HD1 | 1:EB:185:ILE:HD11 | 1.79 | 0.48 |
| 1:EB:209:TRP:HE3 | 1:EB:212:LYS:CB | 2.26 | 0.48 |
| 2:EC:186:ASP:HB3 | 2:EC:189:ARG:NE | 2.28 | 0.48 |
| 2:EC:777:LEU:HD12 | 2:EC:778:THR:H | 1.79 | 0.48 |
| 3:ED:43:ARG:HD2 | 3:ED:74:HIS:CD2 | 2.48 | 0.48 |
| 4:EG:114:GLY:HA3 | 4:EG:143:TYR:CE2 | 2.49 | 0.48 |
| 4:EG:157:THR:O | 4:EG:159:VAL:HG23 | 2.13 | 0.48 |
| 5:EI:253:GLN:HA | 5:EI:390:LEU:HD22 | 1.96 | 0.48 |
| 5:EI:490:TRP:NE1 | 5:EI:515:THR:O | 2.47 | 0.48 |
| 5:EJ:290:SER:CB | 5:EJ:371:PHE:H | 2.27 | 0.48 |
| 5:EJ:48:ALA:O | 5:EJ:49:TRP:HD1 | 1.97 | 0.48 |
| 5:FA:164:ARG:HA | 5:FA:181:PHE:CZ | 2.49 | 0.48 |
| 5:FA:320:LEU:HB3 | 5:FA:358:VAL:HB | 1.95 | 0.48 |
| 5:FA:469:PRO:O | 5:FA:473:MET:N | 2.45 | 0.48 |
| 7:FE:154:ALA:HB3 | 7:FG:162:PRO:HG2 | 1.96 | 0.48 |
| 7:FE:161:THR:O | 7:FE:165:THR:HG22 | 2.13 | 0.48 |
| 7:FG:456:ASP:HA | 7:FG:462:ASN:HD21 | 1.79 | 0.48 |
| 8:FI:10:PHE:CE2 | 8:FI:15:PHE:CE1 | 3.01 | 0.48 |
| 1:GD:210:THR:HG22 | 1:GD:225:TYR:HA | 1.95 | 0.48 |
| 1:GE:129:THR:HG22 | 1:GE:147:SER:HB3 | 1.96 | 0.48 |
| 2:GF:18:ALA:HA | 2:GF:102:THR:HB | 1.94 | 0.48 |
| 2:GF:520:SER:O | 2:GF:522:THR:HG23 | 2.14 | 0.48 |
| 2:GF:85:ALA:HB2 | 2:GF:91:GLN:HE22 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:32:PRO:O | 3:GH:34:LYS:N | 2.47 | 0.48 |
| 4:H:85:HIS:HD2 | 4:H:109:PHE:HE1 | 1.62 | 0.48 |
| 4:HA:200:ALA:HB3 | 4:HA:221:ILE:HD11 | 1.96 | 0.48 |
| 5:HB:354:THR:HG22 | 5:HB:372:ASP:CG | 2.34 | 0.48 |
| 5:HB:496:ASP:HB3 | 5:HB:500:ALA:HB2 | 1.95 | 0.48 |
| 5:HC:192:ARG:HB2 | 5:HC:245:GLU:HB2 | 1.95 | 0.48 |
| 5:HC:48:ALA:C | 5:HC:49:TRP:HD1 | 2.17 | 0.48 |
| 5:HD:469:PRO:O | 5:HD:473:MET:N | 2.45 | 0.48 |
| 5:HD:496:ASP:OD2 | 5:HD:499:PHE:HB2 | 2.13 | 0.48 |
| 6:HE:29:VAL:O | 6:HE:32:ARG:N | 2.36 | 0.48 |
| 6:HE:73:ASN:HB3 | 6:HG:69:THR:HA | 1.96 | 0.48 |
| 6:HG:47:PHE:CZ | 6:HG:49:GLU:HB2 | 2.49 | 0.48 |
| 7:HI:118:PRO:HG3 | 7:HJ:106:ALA:HA | 1.96 | 0.48 |
| 7:HH:339:ARG:NH1 | 7:HJ:356:SER:HB2 | 2.28 | 0.48 |
| 7:HJ:8:HIS:ND1 | 7:HJ:8:HIS:O | 2.46 | 0.48 |
| 8:IA:85:PHE:HB3 | 8:IA:137:VAL:HG21 | 1.96 | 0.48 |
| 11:IE:38:ARG:HH11 | 11:IE:187:ILE:HD12 | 1.78 | 0.48 |
| 12:W:166:SER:OG | 12:IF:16:PHE:N | 2.47 | 0.48 |
| 5:J:166:GLU:OE1 | 5:J:166:GLU:N | 2.47 | 0.48 |
| 5:K:139:ALA:HB3 | 5:K:140:PRO:HD3 | 1.96 | 0.48 |
| 5:K:136:VAL:O | 5:K:143:TRP:HA | 2.14 | 0.48 |
| 5:K:170:GLU:O | 5:K:171:VAL:HG12 | 2.13 | 0.48 |
| 6:L:125:PHE:O | 6:L:129:VAL:HG23 | 2.14 | 0.48 |
| 7:O:176:ILE:HG23 | 7:O:177:ALA:N | 2.28 | 0.48 |
| 7:O:97:LEU:HD23 | 7:Q:97:LEU:HD21 | 1.96 | 0.48 |
| 7:P:424:ARG:O | 7:Q:504:ARG:NH2 | 2.36 | 0.48 |
| 8:R:85:PHE:HB3 | 8:R:137:VAL:HG21 | 1.96 | 0.48 |
| 11:V:61:ASN:O | 11:V:65:GLY:N | 2.38 | 0.48 |
| 12:W:187:GLY:O | 12:W:188:LEU:HD12 | 2.14 | 0.48 |
| 1:X:436:LEU:O | 1:X:439:GLN:N | 2.47 | 0.48 |
| 1:Y:20:ILE:O | 1:Y:22:VAL:HG23 | 2.14 | 0.48 |
| 1:Y:411:PRO:HG2 | 1:Y:413:TYR:HE1 | 1.76 | 0.48 |
| 13:YA:131[F]:VAL:O | 13:YA:134[F]:GLN:N | 2.46 | 0.48 |
| 13:YA:16[F]:GLU:CD | 13:YA:30[F]:ARG:HH11 | 2.17 | 0.48 |
| 13:YA:189[D]:LYS:HA | 13:YA:234[D]:GLY:O | 2.14 | 0.48 |
| 13:YA:370[F]:ASN:ND2 | 13:YA:372[F]:SER:HB3 | 2.29 | 0.48 |
| 13:YA:379[E]:PRO:HG2 | 13:YA:429[E]:ARG:NE | 2.29 | 0.48 |
| 13:YA:453[F]:ASP:OD1 | 13:YC:321[F]:LYS:HG2 | 2.14 | 0.48 |
| 13:YA:554[B]:MET:SD | 13:YA:554[B]:MET:N | 2.86 | 0.48 |
| 13:YA:554[E]:MET:N | 13:YA:554[E]:MET:SD | 2.86 | 0.48 |
| 13:YA:61[A]:ILE:HA | 13:YB:76[A]:PRO:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:189[B]:LYS:HA | 13:YB:234[B]:GLY:O | 2.14 | 0.48 |
| 13:YC:16[F]:GLU:CD | 13:YC:30[F]:ARG:HH11 | 2.17 | 0.48 |
| 13:YC:379[C]:PRO:HG2 | 13:YC:429[C]:ARG:NE | 2.29 | 0.48 |
| 13:YB:460[F]:GLY:HA3 | 13:YC:453[F]:ASP:HA | 1.95 | 0.48 |
| 13:YA:464[C]:TYR:OH | 13:YC:454[C]:LYS:NZ | 2.47 | 0.48 |
| 13:YB:490[E]:VAL:HG11 | 13:YC:486[E]:GLU:CB | 2.43 | 0.48 |
| 13:YC:554[A]:MET:N | 13:YC:554[A]:MET:SD | 2.86 | 0.48 |
| 13:YA:60[B]:PRO:HD2 | 13:YC:61[B]:ILE:HG12 | 1.96 | 0.48 |
| 13:YA:388[B]:PRO:HB2 | 13:YC:74[B]:THR:HG21 | 1.95 | 0.48 |
| 14:YD:54[C]:PHE:CZ | 14:YD:105[C]:ILE:HD11 | 2.49 | 0.48 |
| 14:YD:214[D]:GLY:O | 14:YD:215[D]:GLU:HG3 | 2.14 | 0.48 |
| 14:YD:254[A]:TYR:CD2 | 14:YD:265[A]:MET:HG2 | 2.49 | 0.48 |
| 13:YB:44[D]:VAL:HG11 | 14:YD:272[D]:GLU:HB3 | 1.95 | 0.48 |
| 14:YD:31[F]:LEU:O | 14:YD:35[F]:ILE:HG22 | 2.14 | 0.48 |
| 14:YD:328[C]:ASP:OD1 | 14:YD:329[C]:SER:N | 2.47 | 0.48 |
| 14:YD:328[A]:ASP:OD1 | 14:YD:329[A]:SER:N | 2.47 | 0.48 |
| 14:YD:310[B]:CYS:SG | 14:YD:355[B]:LEU:HB2 | 2.54 | 0.48 |
| 14:YD:97[B]:VAL:HG12 | 14:YF:234[B]:PHE:HD1 | 1.79 | 0.48 |
| 14:YD:97[D]:VAL:HG21 | 14:YF:332[D]:GLN:NE2 | 2.29 | 0.48 |
| 14:YE:278[D]:SER:O | 14:YE:279[D]:ARG:NH1 | 2.44 | 0.48 |
| 14:YE:31[D]:LEU:O | 14:YE:35[D]:ILE:HG22 | 2.14 | 0.48 |
| 14:YE:328[B]:ASP:OD1 | 14:YE:329[B]:SER:N | 2.47 | 0.48 |
| 10:ID:286:VAL:HG13 | 14:YF:100[D]:LYS:HE2 | 1.96 | 0.48 |
| 14:YF:185[D]:PHE:CD2 | 14:YF:297[D]:ARG:HA | 2.49 | 0.48 |
| 14:YF:254[A]:TYR:CD2 | 14:YF:265[A]:MET:HG2 | 2.49 | 0.48 |
| 14:YF:328[C]:ASP:OD1 | 14:YF:329[C]:SER:N | 2.47 | 0.48 |
| 14:YF:328[D]:ASP:OD1 | 14:YF:329[D]:SER:N | 2.47 | 0.48 |
| 14:YF:328[E]:ASP:OD1 | 14:YF:329[E]:SER:N | 2.47 | 0.48 |
| 14:YF:304[F]:TYR:HB3 | 14:YF:358[F]:PHE:HD1 | 1.78 | 0.48 |
| 14:YF:54[D]:PHE:CZ | 14:YF:105[D]:ILE:HD11 | 2.49 | 0.48 |
| 14:YF:54[E]:PHE:CZ | 14:YF:105[E]:ILE:HD11 | 2.49 | 0.48 |
| 14:YF:54[F]:PHE:CZ | 14:YF:105[F]:ILE:HD11 | 2.49 | 0.48 |
| 2:Z:784:GLN:HG2 | 2:Z:830:ARG:HG2 | 1.96 | 0.48 |
| 4:AA:172:GLU:HA | 4:AB:166:SER:H | 1.79 | 0.47 |
| 4:AA:53:GLY:O | 4:AB:7:LYS:HB3 | 2.14 | 0.47 |
| 5:AD:170:GLU:O | 5:AD:171:VAL:HG12 | 2.14 | 0.47 |
| 5:AC:591:PRO:HA | 5:AD:520:GLY:O | 2.14 | 0.47 |
| 5:AD:67:SER:CB | 5:AD:94:ARG:HB2 | 2.44 | 0.47 |
| 5:AD:49:TRP:HZ3 | 5:AD:96:ARG:CD | 2.26 | 0.47 |
| 5:AE:164:ARG:HA | 5:AE:181:PHE:HZ | 1.79 | 0.47 |
| 5:AE:86:VAL:HG13 | 5:AE:87:ASN:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:367:VAL:O | 7:AI:389:ASN:HA | 2.13 | 0.47 |
| 7:AJ:117:THR:OG1 | 7:BA:112:ASN:HA | 2.14 | 0.47 |
| 1:BH:130:ARG:HD3 | 14:YF:181[F]:GLY:HA2 | 1.94 | 0.47 |
| 1:BH:200:TYR:HB2 | 1:BH:269:VAL:CG1 | 2.44 | 0.47 |
| 1:BH:402:ALA:N | 1:BH:403:PRO:HD2 | 2.29 | 0.47 |
| 2:BJ:555:ARG:HD2 | 2:BJ:557:VAL:O | 2.14 | 0.47 |
| 2:C:229:VAL:O | 2:C:249:GLY:HA2 | 2.14 | 0.47 |
| 2:C:231:TYR:CE1 | 2:C:391:ARG:HD3 | 2.48 | 0.47 |
| 2:C:555:ARG:HG3 | 2:C:557:VAL:N | 2.29 | 0.47 |
| 2:C:853:ASP:OD1 | 2:C:854:TYR:N | 2.47 | 0.47 |
| 2:C:926:PRO:HG2 | 2:C:985:GLU:HG2 | 1.94 | 0.47 |
| 4:CD:157:THR:O | 4:CD:159:VAL:HG23 | 2.13 | 0.47 |
| 4:CD:218:GLU:OE1 | 4:CE:201:LYS:NZ | 2.37 | 0.47 |
| 4:CE:200:ALA:HB3 | 4:CE:221:ILE:HD11 | 1.96 | 0.47 |
| 5:CG:34:TYR:O | 5:CG:38:GLY:N | 2.37 | 0.47 |
| 5:CH:396:LYS:O | 5:CH:399:ILE:HG13 | 2.14 | 0.47 |
| 5:CH:430:TRP:CZ2 | 5:CH:433:VAL:HG11 | 2.49 | 0.47 |
| 6:CI:47:PHE:CZ | 6:CI:49:GLU:HB2 | 2.49 | 0.47 |
| 7:DB:246:THR:HG1 | 7:DB:249:THR:H | 1.61 | 0.47 |
| 7:DB:477:TRP:CZ3 | 7:DC:469:VAL:HB | 2.49 | 0.47 |
| 7:DC:142:ILE:HG22 | 7:DC:143:LYS:O | 2.14 | 0.47 |
| 7:DD:142:ILE:HG22 | 7:DD:143:LYS:N | 2.29 | 0.47 |
| 7:DC:227:VAL:HG23 | 7:DD:225:LYS:HD3 | 1.95 | 0.47 |
| 12:DJ:158:LEU:HD21 | 12:DJ:216:PHE:CE1 | 2.48 | 0.47 |
| 1:EB:20:ILE:O | 1:EB:22:VAL:HG23 | 2.14 | 0.47 |
| 1:EB:231:ASP:OD1 | 1:EB:232:GLY:N | 2.46 | 0.47 |
| 1:EB:45:ASP:C | 1:EB:47:ASP:H | 2.10 | 0.47 |
| 2:EC:196:GLU:HG2 | 2:EC:197:GLY:N | 2.29 | 0.47 |
| 2:EC:520:SER:O | 2:EC:522:THR:HG23 | 2.14 | 0.47 |
| 2:EC:986:ARG:HH22 | 3:ED:323:ASP:HB2 | 1.78 | 0.47 |
| 4:EH:200:ALA:HB3 | 4:EH:221:ILE:HD11 | 1.96 | 0.47 |
| 5:EJ:132:ASP:N | 5:EJ:149:LYS:O | 2.47 | 0.47 |
| 5:EJ:170:GLU:O | 5:EJ:171:VAL:HG12 | 2.14 | 0.47 |
| 5:EI:569:TYR:N | 5:EJ:550:VAL:HB | 2.29 | 0.47 |
| 5:EJ:319:GLU:HG3 | 5:FA:262:GLN:OE1 | 2.13 | 0.47 |
| 5:FA:335:ASP:N | 5:FA:335:ASP:OD1 | 2.47 | 0.47 |
| 2:EC:995:ASP:HB2 | 5:FA:7:ILE:HG22 | 1.95 | 0.47 |
| 5:EI:318:GLN:HB3 | 6:FD:4:LEU:CD1 | 2.44 | 0.47 |
| 7:FE:97:LEU:HD23 | 7:FG:97:LEU:HD21 | 1.96 | 0.47 |
| 7:FG:142:ILE:HG22 | 7:FG:143:LYS:N | 2.29 | 0.47 |
| 7:FE:469:VAL:HB | 7:FG:477:TRP:CZ3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:FJ:18:ASP:OD1 | 9:FJ:19:TRP:N | 2.46 | 0.47 |
| 12:GC:16:PHE:N | 12:IF:166:SER:OG | 2.47 | 0.47 |
| 1:GD:200:TYR:HB2 | 1:GD:269:VAL:CG1 | 2.44 | 0.47 |
| 1:GD:484:MET:HG2 | 1:GD:627:PRO:HD3 | 1.95 | 0.47 |
| 2:GF:189:ARG:HD3 | 2:GF:203:GLU:OE2 | 2.14 | 0.47 |
| 3:GH:13:THR:HG22 | 3:GH:15:LYS:H | 1.78 | 0.47 |
| 4:GI:200:ALA:HB3 | 4:GI:221:ILE:HD11 | 1.96 | 0.47 |
| 4:HA:107:VAL:O | 4:HA:148:LEU:N | 2.39 | 0.47 |
| 4:HA:30:LYS:O | 4:HA:34:ASP:N | 2.45 | 0.47 |
| 5:HD:170:GLU:O | 5:HD:171:VAL:HG12 | 2.13 | 0.47 |
| 6:HF:47:PHE:CZ | 6:HF:49:GLU:HB2 | 2.49 | 0.47 |
| 6:HG:127:ALA:HA | 6:HG:130:ARG:HH11 | 1.79 | 0.47 |
| 7:HH:321:MET:HA | 7:HJ:315:ILE:O | 2.15 | 0.47 |
| 7:HI:117:THR:OG1 | 7:HJ:112:ASN:HA | 2.14 | 0.47 |
| 7:HH:479:ASN:O | 7:HI:468:PHE:HB2 | 2.13 | 0.47 |
| 7:HI:227:VAL:HG23 | 7:HJ:225:LYS:HD3 | 1.95 | 0.47 |
| 7:HH:329:ASN:CG | 7:HJ:333:THR:HB | 2.34 | 0.47 |
| 5:I:253:GLN:HA | 5:I:390:LEU:HD22 | 1.96 | 0.47 |
| 5:I:354:THR:HG22 | 5:I:372:ASP:CG | 2.34 | 0.47 |
| 5:I:89:TYR:O | 5:I:91:LYS:HG2 | 2.13 | 0.47 |
| 10:ID:142:ARG:O | 10:ID:143:PHE:HD1 | 1.96 | 0.47 |
| 11:IE:14:LYS:HE2 | 11:IE:19:ASN:HA | 1.96 | 0.47 |
| 11:IE:74:LEU:HD11 | 11:IE:79:ASN:HD21 | 1.79 | 0.47 |
| 5:K:190:ASN:HB2 | 5:K:247:PHE:HB2 | 1.95 | 0.47 |
| 5:J:357:SER:OG | 6:L:4:LEU:HD21 | 2.14 | 0.47 |
| 6:L:32:ARG:NH1 | 6:M:144:ASN:OD1 | 2.43 | 0.47 |
| 6:M:54:SER:HA | 6:N:164:GLN:HE22 | 1.78 | 0.47 |
| 7:O:493:GLU:HG3 | 7:O:496:ARG:HH21 | 1.79 | 0.47 |
| 7:P:54:THR:HG22 | 7:P:55:LYS:O | 2.13 | 0.47 |
| 7:P:100:TYR:OH | 7:Q:113:GLU:O | 2.05 | 0.47 |
| 7:Q:253:ARG:O | 7:Q:262:VAL:HG22 | 2.14 | 0.47 |
| 7:O:504:ARG:HA | 7:Q:422:LYS:HB3 | 1.95 | 0.47 |
| 11:V:94:TYR:CE1 | 11:V:156:TYR:HB3 | 2.49 | 0.47 |
| 11:V:38:ARG:HH11 | 11:V:187:ILE:HD12 | 1.78 | 0.47 |
| 11:V:74:LEU:HD11 | 11:V:79:ASN:HD21 | 1.79 | 0.47 |
| 12:W:241:VAL:HG13 | 12:W:241:VAL:O | 2.14 | 0.47 |
| 1:X:112:LEU:HD13 | 1:X:297:VAL:HG12 | 1.96 | 0.47 |
| 1:X:145:PHE:HZ | 1:X:286:PHE:CE1 | 2.32 | 0.47 |
| 1:Y:205:GLU:O | 1:Y:206:TRP:HD1 | 1.97 | 0.47 |
| 13:YA:12[E]:VAL:HG21 | 14:YF:256[E]:HIS:CE1 | 2.49 | 0.47 |
| 13:YA:189[B]:LYS:HA | 13:YA:234[B]:GLY:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:307[D]:ALA:HB1 | 13:YA:331[D]:ILE:HD11 | 1.95 | 0.47 |
| 13:YB:147[E]:ILE:O | 13:YB:151[E]:ASN:ND2 | 2.47 | 0.47 |
| 13:YB:307[B]:ALA:HB1 | 13:YB:331[B]:ILE:HD11 | 1.95 | 0.47 |
| 13:YB:387[D]:TYR:CE1 | 13:YB:388[D]:PRO:HB3 | 2.49 | 0.47 |
| 13:YB:387[F]:TYR:CE1 | 13:YB:388[F]:PRO:HB3 | 2.49 | 0.47 |
| 13:YB:546[E]:VAL:HA | 13:YC:538[E]:VAL:O | 2.14 | 0.47 |
| 13:YB:66[B]:MET:HE2 | 13:YC:122[B]:PRO:HB3 | 1.96 | 0.47 |
| 13:YC:131[B]:VAL:O | 13:YC:134[B]:GLN:N | 2.47 | 0.47 |
| 13:YC:189[F]:LYS:HA | 13:YC:234[F]:GLY:O | 2.14 | 0.47 |
| 13:YC:189[D]:LYS:HA | 13:YC:234[D]:GLY:O | 2.14 | 0.47 |
| 13:YA:453[B]:ASP:OD1 | 13:YC:321[B]:LYS:HG2 | 2.14 | 0.47 |
| 13:YB:158[C]:PRO:HB2 | 13:YC:473[C]:GLN:OE1 | 2.14 | 0.47 |
| 13:YA:122[E]:PRO:HB3 | 13:YC:66[E]:MET:HE2 | 1.95 | 0.47 |
| 14:YD:31[E]:LEU:O | 14:YD:35[E]:ILE:HG22 | 2.14 | 0.47 |
| 14:YE:14[B]:VAL:HG11 | 14:YE:52[B]:LEU:HD11 | 1.96 | 0.47 |
| 14:YE:214[C]:GLY:O | 14:YE:215[C]:GLU:HG3 | 2.14 | 0.47 |
| 10:ID:285:LEU:HA | 14:YE:215[D]:GLU:HG2 | 1.92 | 0.47 |
| 14:YE:301[B]:MET:HA | 14:YE:304[B]:TYR:CD2 | 2.47 | 0.47 |
| 14:YE:310[B]:CYS:SG | 14:YE:355[B]:LEU:HB2 | 2.54 | 0.47 |
| 14:YE:328[D]:ASP:OD1 | 14:YE:329[D]:SER:N | 2.47 | 0.47 |
| 14:YE:328[E]:ASP:OD1 | 14:YE:329[E]:SER:N | 2.47 | 0.47 |
| 14:YE:332[A]:GLN:HB3 | 14:YF:61[A]:HIS:NE2 | 2.29 | 0.47 |
| 14:YE:304[C]:TYR:HB3 | 14:YE:358[C]:PHE:HD1 | 1.78 | 0.47 |
| 14:YE:31[F]:LEU:O | 14:YE:35[F]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:14[F]:VAL:HG11 | 14:YF:52[F]:LEU:HD11 | 1.96 | 0.47 |
| 14:YF:185[A]:PHE:CD2 | 14:YF:297[A]:ARG:HA | 2.49 | 0.47 |
| 14:YF:185[E]:PHE:CD2 | 14:YF:297[E]:ARG:HA | 2.49 | 0.47 |
| 14:YF:185[F]:PHE:CD2 | 14:YF:297[F]:ARG:HA | 2.49 | 0.47 |
| 14:YF:214[D]:GLY:O | 14:YF:215[D]:GLU:HG3 | 2.14 | 0.47 |
| 14:YF:310[F]:CYS:SG | 14:YF:355[F]:LEU:HB2 | 2.54 | 0.47 |
| 14:YF:328[F]:ASP:OD1 | 14:YF:329[F]:SER:N | 2.47 | 0.47 |
| 14:YF:31[B]:LEU:O | 14:YF:35[B]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:72[E]:ILE:O | 14:YF:86[E]:ARG:N | 2.47 | 0.47 |
| 2:Z:103:PHE:CZ | 2:Z:626:GLN:O | 2.64 | 0.47 |
| 2:Z:193:MET:O | 2:Z:200:TYR:N | 2.36 | 0.47 |
| 2:Z:319:TYR:CD1 | 2:Z:328:TYR:HB2 | 2.47 | 0.47 |
| 2:Z:339:ASP:O | 2:Z:341:LEU:N | 2.47 | 0.47 |
| 1:A:5:PRO:HG3 | 1:A:36:TRP:CZ2 | 2.49 | 0.47 |
| 1:A:377:LYS:CD | 1:A:641:VAL:HG21 | 2.43 | 0.47 |
| 4:AB:107:VAL:O | 4:AB:148:LEU:N | 2.39 | 0.47 |
| 5:AC:253:GLN:HA | 5:AC:390:LEU:HD22 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:202:TYR:CZ | 5:AE:225:LEU:HB2 | 2.49 | 0.47 |
| 5:AD:591:PRO:HA | 5:AE:520:GLY:O | 2.14 | 0.47 |
| 6:AH:125:PHE:O | 6:AH:129:VAL:HG23 | 2.14 | 0.47 |
| 7:BA:142:ILE:HG22 | 7:BA:143:LYS:N | 2.29 | 0.47 |
| 7:BA:31:ASP:CG | 7:BA:34:ALA:H | 2.17 | 0.47 |
| 1:BH:436:LEU:O | 1:BH:439:GLN:N | 2.47 | 0.47 |
| 2:BJ:339:ASP:O | 2:BJ:341:LEU:N | 2.47 | 0.47 |
| 2:BJ:454:ASN:HB2 | 2:BJ:471:VAL:HG21 | 1.96 | 0.47 |
| 2:BJ:543:LYS:HE2 | 2:BJ:574:LYS:O | 2.14 | 0.47 |
| 2:BJ:821:ILE:O | 2:BJ:824:GLN:NE2 | 2.32 | 0.47 |
| 2:C:494:GLU:HB2 | 2:C:498:TRP:HB2 | 1.96 | 0.47 |
| 2:C:85:ALA:HB2 | 2:C:91:GLN:HE22 | 1.79 | 0.47 |
| 3:CA:46:PRO:HB3 | 3:CA:51:GLU:OE2 | 2.13 | 0.47 |
| 3:CA:64:SER:OG | 3:CA:67:GLY:N | 2.35 | 0.47 |
| 4:CC:200:ALA:HB3 | 4:CC:221:ILE:HD11 | 1.96 | 0.47 |
| 4:CE:212:ARG:HG3 | 4:CE:213:LYS:HG3 | 1.96 | 0.47 |
| 5:CF:259:THR:OG1 | 5:CF:385:TRP:HB2 | 2.14 | 0.47 |
| 5:CG:247:PHE:HZ | 5:CH:162:VAL:HG21 | 1.78 | 0.47 |
| 5:CG:48:ALA:O | 5:CG:49:TRP:HD1 | 1.97 | 0.47 |
| 5:CG:506:LEU:HD23 | 5:CG:512:PRO:HA | 1.96 | 0.47 |
| 5:CF:196:ARG:HG2 | 5:CH:198:ASN:O | 2.14 | 0.47 |
| 5:CH:358:VAL:HG23 | 5:CH:371:PHE:HD1 | 1.78 | 0.47 |
| 6:CJ:125:PHE:O | 6:CJ:129:VAL:HG23 | 2.14 | 0.47 |
| 6:DA:125:PHE:O | 6:DA:129:VAL:HG23 | 2.14 | 0.47 |
| 6:DA:29:VAL:O | 6:DA:32:ARG:N | 2.36 | 0.47 |
| 7:DC:141:VAL:HG22 | 7:DD:139:ASN:HB2 | 1.96 | 0.47 |
| 7:DC:516:ASN:ND2 | 7:DD:401:ARG:HD2 | 2.29 | 0.47 |
| 7:DD:160:MET:HG2 | 7:DD:165:THR:HB | 1.96 | 0.47 |
| 7:DD:325:TYR:CD1 | 7:DD:330:ARG:HA | 2.45 | 0.47 |
| 7:DD:456:ASP:HA | 7:DD:462:ASN:HD21 | 1.79 | 0.47 |
| 8:DF:85:PHE:HB3 | 8:DF:137:VAL:HG21 | 1.96 | 0.47 |
| 10:DH:205:LYS:HB2 | 10:DH:311:PHE:CZ | 2.49 | 0.47 |
| 3:E:221:THR:O | 3:E:224:GLY:N | 2.37 | 0.47 |
| 1:EA:112:LEU:HD13 | 1:EA:297:VAL:HG12 | 1.96 | 0.47 |
| 1:EB:129:THR:HG22 | 1:EB:147:SER:HB3 | 1.96 | 0.47 |
| 1:EB:143:TYR:CD2 | 1:EB:279:ASP:HB2 | 2.49 | 0.47 |
| 2:EC:20:GLN:HG2 | 2:EC:70:ASP:CG | 2.33 | 0.47 |
| 2:EC:923:SER:HB3 | 2:EC:992:PRO:HG2 | 1.96 | 0.47 |
| 3:ED:195:PRO:HB2 | 3:ED:197:ASP:OD1 | 2.14 | 0.47 |
| 3:ED:38:PHE:CD1 | 3:ED:80:LYS:HA | 2.49 | 0.47 |
| 3:ED:46:PRO:HB3 | 3:ED:51:GLU:OE2 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:EE:13:THR:HG22 | 3:EE:15:LYS:H | 1.78 | 0.47 |
| 3:EE:47:TRP:CD1 | 3:EE:270:ARG:HD2 | 2.50 | 0.47 |
| 5:EI:117:ILE:HG22 | 5:EI:143:TRP:HE3 | 1.79 | 0.47 |
| 6:FC:127:ALA:HA | 6:FC:130:ARG:HH11 | 1.79 | 0.47 |
| 7:FE:170:ILE:HA | 7:FE:173:ILE:HG22 | 1.95 | 0.47 |
| 7:FE:329:ASN:HD21 | 7:FG:335:ASN:H | 1.62 | 0.47 |
| 8:FH:85:PHE:HB3 | 8:FH:137:VAL:HG21 | 1.96 | 0.47 |
| 8:DF:117:ALA:HA | 8:FI:77:GLU:OE2 | 2.14 | 0.47 |
| 9:FJ:58:SER:O | 9:FJ:62:PHE:N | 2.34 | 0.47 |
| 11:GB:135:ASP:CG | 11:GB:136:LYS:N | 2.67 | 0.47 |
| 11:GB:146:TYR:CE2 | 11:GB:150:LEU:HD23 | 2.48 | 0.47 |
| 11:GB:74:LEU:HD11 | 11:GB:79:ASN:HD21 | 1.79 | 0.47 |
| 12:GC:126:TYR:HA | 12:IF:230:TYR:HD2 | 1.75 | 0.47 |
| 1:GD:634:THR:HB | 1:GD:638:SER:O | 2.14 | 0.47 |
| 1:GD:636:ASP:N | 1:GD:636:ASP:OD1 | 2.44 | 0.47 |
| 1:GE:118:LEU:HG | 1:GE:294:ASN:CG | 2.35 | 0.47 |
| 1:GE:485:VAL:HG11 | 1:GE:650:TYR:HE1 | 1.79 | 0.47 |
| 2:GF:1025:PRO:C | 2:GF:1027:GLN:H | 2.17 | 0.47 |
| 2:GF:454:ASN:HB2 | 2:GF:471:VAL:HG21 | 1.96 | 0.47 |
| 3:E:241:ARG:HH12 | 2:GF:483:LYS:HE2 | 1.78 | 0.47 |
| 2:GF:643:PRO:HG2 | 11:IE:84:TYR:CE2 | 2.49 | 0.47 |
| 4:GI:114:GLY:HA3 | 4:GI:143:TYR:CE2 | 2.49 | 0.47 |
| 4:GI:7:LYS:HE2 | 4:HA:53:GLY:HA3 | 1.96 | 0.47 |
| 4:H:114:GLY:HA3 | 4:H:143:TYR:CE2 | 2.49 | 0.47 |
| 4:H:200:ALA:HB3 | 4:H:221:ILE:HD11 | 1.96 | 0.47 |
| 4:H:50:VAL:C | 4:H:52:ASN:H | 2.17 | 0.47 |
| 4:HA:157:THR:O | 4:HA:159:VAL:HG23 | 2.13 | 0.47 |
| 5:HB:490:TRP:NE1 | 5:HB:515:THR:O | 2.47 | 0.47 |
| 5:HC:304:ILE:HG21 | 5:HC:309:LEU:HD12 | 1.96 | 0.47 |
| 5:HD:136:VAL:O | 5:HD:143:TRP:HA | 2.14 | 0.47 |
| 6:HE:47:PHE:CZ | 6:HE:49:GLU:HB2 | 2.49 | 0.47 |
| 7:HH:154:ALA:HB3 | 7:HJ:162:PRO:HG2 | 1.96 | 0.47 |
| 7:HI:141:VAL:HG22 | 7:HJ:139:ASN:HB2 | 1.95 | 0.47 |
| 7:HJ:142:ILE:HG22 | 7:HJ:143:LYS:N | 2.29 | 0.47 |
| 7:HJ:31:ASP:CG | 7:HJ:34:ALA:H | 2.18 | 0.47 |
| 7:HH:76:VAL:N | 7:HJ:76:VAL:O | 2.34 | 0.47 |
| 12:GC:149:ARG:HB3 | 10:ID:212:THR:HG21 | 1.94 | 0.47 |
| 11:IE:94:TYR:CE1 | 11:IE:156:TYR:HB3 | 2.49 | 0.47 |
| 12:IF:241:VAL:HG13 | 12:IF:241:VAL:O | 2.14 | 0.47 |
| 5:J:304:ILE:HG21 | 5:J:309:LEU:HD12 | 1.96 | 0.47 |
| 5:J:320:LEU:HG | 5:J:357:SER:CB | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:48:ALA:C | 5:J:49:TRP:HD1 | 2.17 | 0.47 |
| 5:J:507:ASP:OD2 | 5:J:511:ASN:HB2 | 2.14 | 0.47 |
| 5:K:63:GLU:HB2 | 5:K:68:TYR:OH | 2.14 | 0.47 |
| 7:O:321:MET:HA | 7:Q:315:ILE:O | 2.14 | 0.47 |
| 7:P:151:LEU:HD12 | 7:P:171:LYS:HE2 | 1.95 | 0.47 |
| 7:Q:476:ASP:O | 7:Q:479:ASN:ND2 | 2.47 | 0.47 |
| 10:U:205:LYS:HB2 | 10:U:311:PHE:CZ | 2.49 | 0.47 |
| 13:YA:189[E]:LYS:HA | 13:YA:234[E]:GLY:O | 2.14 | 0.47 |
| 13:YA:379[F]:PRO:HG2 | 13:YA:429[F]:ARG:NE | 2.29 | 0.47 |
| 13:YB:147[F]:ILE:O | 13:YB:151[F]:ASN:ND2 | 2.47 | 0.47 |
| 13:YB:387[A]:TYR:CE1 | 13:YB:388[A]:PRO:HB3 | 2.49 | 0.47 |
| 13:YB:554[C]:MET:N | 13:YB:554[C]:MET:SD | 2.86 | 0.47 |
| 13:YA:571[D]:ARG:HD3 | 13:YB:564[D]:GLN:HE22 | 1.80 | 0.47 |
| 13:YB:24[E]:LEU:HD21 | 13:YC:102[E]:GLY:HA2 | 1.96 | 0.47 |
| 13:YA:453[D]:ASP:OD1 | 13:YC:321[D]:LYS:HG2 | 2.14 | 0.47 |
| 13:YC:370[A]:ASN:ND2 | 13:YC:372[A]:SER:HB3 | 2.29 | 0.47 |
| 13:YA:447[A]:ASN:HB3 | 13:YC:376[A]:PHE:CE2 | 2.49 | 0.47 |
| 13:YB:474[C]:ILE:HD13 | 13:YC:470[C]:ARG:HB2 | 1.95 | 0.47 |
| 13:YC:57[E]:VAL:HG21 | 13:YC:75[E]:GLY:HA2 | 1.95 | 0.47 |
| 14:YD:185[B]:PHE:CD2 | 14:YD:297[B]:ARG:HA | 2.49 | 0.47 |
| 14:YD:185[C]:PHE:CD2 | 14:YD:297[C]:ARG:HA | 2.49 | 0.47 |
| 14:YD:185[E]:PHE:CD2 | 14:YD:297[E]:ARG:HA | 2.49 | 0.47 |
| 14:YD:214[B]:GLY:O | 14:YD:215[B]:GLU:HG3 | 2.14 | 0.47 |
| 14:YD:301[D]:MET:HA | 14:YD:304[D]:TYR:CD2 | 2.47 | 0.47 |
| 14:YD:328[F]:ASP:OD1 | 14:YD:329[F]:SER:N | 2.47 | 0.47 |
| 14:YD:61[C]:HIS:NE2 | 14:YF:332[C]:GLN:HB3 | 2.28 | 0.47 |
| 14:YD:72[C]:ILE:O | 14:YD:86[C]:ARG:N | 2.47 | 0.47 |
| 14:YE:252[B]:THR:OG1 | 14:YE:271[B]:GLY:O | 2.32 | 0.47 |
| 14:YE:310[F]:CYS:SG | 14:YE:355[F]:LEU:HB2 | 2.54 | 0.47 |
| 14:YE:336[B]:GLU:O | 14:YE:359[B]:THR:OG1 | 2.33 | 0.47 |
| 14:YF:301[F]:MET:HA | 14:YF:304[F]:TYR:CD2 | 2.47 | 0.47 |
| 2:Z:934:ALA:H | 2:Z:997:SER:HB2 | 1.79 | 0.47 |
| 2:Z:946:SER:OG | 2:Z:947:VAL:HG13 | 2.14 | 0.47 |
| 1:A:448:TYR:HA | 1:A:452:VAL:HG12 | 1.95 | 0.47 |
| 4:AB:114:GLY:HA3 | 4:AB:143:TYR:CE2 | 2.49 | 0.47 |
| 5:AC:182:ARG:HH22 | 5:AD:299:ILE:HG21 | 1.80 | 0.47 |
| 5:AE:157:SER:O | 5:AE:160:SER:OG | 2.28 | 0.47 |
| 6:AG:47:PHE:CZ | 6:AG:49:GLU:HB2 | 2.49 | 0.47 |
| 6:AH:76:GLY:HA2 | 6:AH:215:PHE:HZ | 1.79 | 0.47 |
| 7:AJ:368:SER:HA | 7:AJ:389:ASN:HD22 | 1.79 | 0.47 |
| 1:B:129:THR:HG22 | 1:B:147:SER:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:231:ASP:OD1 | 1:B:232:GLY:N | 2.47 | 0.47 |
| 1:B:485:VAL:HG11 | 1:B:650:TYR:HE1 | 1.79 | 0.47 |
| 7:BA:110:VAL:HG12 | 7:BA:111:ASN:N | 2.28 | 0.47 |
| 12:BG:110:LEU:HG | 12:BG:177:TRP:HD1 | 1.79 | 0.47 |
| 1:BH:116:ASP:OD1 | 1:BH:118:LEU:N | 2.46 | 0.47 |
| 1:BH:484:MET:HG2 | 1:BH:627:PRO:HD3 | 1.95 | 0.47 |
| 1:BI:143:TYR:CD2 | 1:BI:279:ASP:HB2 | 2.50 | 0.47 |
| 1:BI:522:LYS:HD2 | 1:BI:530:LEU:HD13 | 1.95 | 0.47 |
| 2:BJ:189:ARG:HD3 | 2:BJ:203:GLU:OE2 | 2.14 | 0.47 |
| 2:BJ:340:PRO:O | 2:BJ:342:SER:N | 2.47 | 0.47 |
| 2:BJ:357:ILE:HG23 | 2:BJ:358:THR:N | 2.30 | 0.47 |
| 2:BJ:698:GLU:HG3 | 2:BJ:699:HIS:N | 2.30 | 0.47 |
| 2:BJ:784:GLN:HG2 | 2:BJ:830:ARG:HG2 | 1.96 | 0.47 |
| 2:C:1000:THR:HG23 | 5:I:17:ASP:O | 2.13 | 0.47 |
| 2:C:213:ASN:HB2 | 2:C:289:PHE:CE1 | 2.50 | 0.47 |
| 2:C:415:ARG:HH22 | 2:C:424:ARG:NH1 | 2.11 | 0.47 |
| 2:C:840:ARG:NH2 | 2:C:843:LYS:HG2 | 2.28 | 0.47 |
| 2:C:923:SER:HB3 | 2:C:992:PRO:HG2 | 1.96 | 0.47 |
| 3:CA:225:TYR:HE2 | 3:CA:231:TRP:HB3 | 1.79 | 0.47 |
| 3:CA:233:GLN:HB2 | 3:CB:289:ASN:HD21 | 1.78 | 0.47 |
| 4:CE:202:LEU:HD21 | 4:CE:254:PHE:CZ | 2.50 | 0.47 |
| 5:CF:591:PRO:HA | 5:CG:520:GLY:O | 2.14 | 0.47 |
| 5:CG:132:ASP:N | 5:CG:149:LYS:O | 2.47 | 0.47 |
| 5:CG:304:ILE:HG21 | 5:CG:309:LEU:HD12 | 1.96 | 0.47 |
| 5:CG:360:THR:HG22 | 5:CG:366:PRO:HG3 | 1.96 | 0.47 |
| 5:CG:290:SER:CB | 5:CG:371:PHE:H | 2.27 | 0.47 |
| 5:CH:164:ARG:HA | 5:CH:181:PHE:HZ | 1.79 | 0.47 |
| 5:CH:469:PRO:O | 5:CH:473:MET:N | 2.45 | 0.47 |
| 7:DD:220:SER:HB2 | 7:DD:228:ILE:HG12 | 1.97 | 0.47 |
| 7:DD:253:ARG:O | 7:DD:262:VAL:HG22 | 2.14 | 0.47 |
| 7:DB:321:MET:HA | 7:DD:315:ILE:O | 2.14 | 0.47 |
| 8:DF:10:PHE:CE2 | 8:DF:15:PHE:CE1 | 3.01 | 0.47 |
| 10:DH:289:ASN:HB2 | 10:DH:290:PRO:HD2 | 1.95 | 0.47 |
| 3:E:13:THR:HG22 | 3:E:15:LYS:H | 1.78 | 0.47 |
| 1:EA:411:PRO:HG2 | 1:EA:413:TYR:HD2 | 1.77 | 0.47 |
| 1:EB:179:TYR:CD1 | 1:EB:185:ILE:HD11 | 2.49 | 0.47 |
| 1:EB:118:LEU:HG | 1:EB:294:ASN:CG | 2.35 | 0.47 |
| 2:EC:357:ILE:HG23 | 2:EC:358:THR:N | 2.30 | 0.47 |
| 2:EC:698:GLU:HG3 | 2:EC:699:HIS:N | 2.30 | 0.47 |
| 2:EC:946:SER:OG | 2:EC:947:VAL:HG13 | 2.14 | 0.47 |
| 2:EC:968:ASP:HB3 | 2:EC:972:GLU:CG | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:246:THR:HA | 3:ED:332:PHE:O | 2.15 | 0.47 |
| 3:EE:193:GLU:HG2 | 3:EE:224:GLY:HA3 | 1.95 | 0.47 |
| 3:EE:71:MET:HG3 | 3:EE:271:GLN:NE2 | 2.29 | 0.47 |
| 5:EI:182:ARG:NH2 | 5:EJ:299:ILE:HG21 | 2.29 | 0.47 |
| 5:EI:316:ILE:HG22 | 5:EI:318:GLN:HG3 | 1.97 | 0.47 |
| 5:EI:402:GLU:HG3 | 5:EI:406:LEU:HD11 | 1.96 | 0.47 |
| 5:EI:518:GLY:N | 5:FA:594:THR:OG1 | 2.48 | 0.47 |
| 5:EJ:335:ASP:N | 5:EJ:335:ASP:OD1 | 2.45 | 0.47 |
| 4:F:202:LEU:HD21 | 4:F:254:PHE:CZ | 2.50 | 0.47 |
| 5:FA:396:LYS:O | 5:FA:399:ILE:HG13 | 2.14 | 0.47 |
| 5:FA:430:TRP:CZ2 | 5:FA:433:VAL:HG11 | 2.49 | 0.47 |
| 5:FA:496:ASP:OD2 | 5:FA:499:PHE:HB2 | 2.13 | 0.47 |
| 5:FA:96:ARG:NH1 | 5:FA:132:ASP:OD2 | 2.48 | 0.47 |
| 6:FC:10:VAL:CA | 6:FD:13:ARG:HD2 | 2.32 | 0.47 |
| 7:FE:160:MET:HG3 | 7:FE:164:LYS:NZ | 2.29 | 0.47 |
| 7:FE:228:ILE:O | 7:FF:220:SER:OG | 2.16 | 0.47 |
| 4:G:212:ARG:HG3 | 4:G:213:LYS:HG3 | 1.96 | 0.47 |
| 12:GC:110:LEU:HG | 12:GC:177:TRP:HD1 | 1.79 | 0.47 |
| 1:GD:224:TYR:HA | 1:GD:238:PHE:HB3 | 1.96 | 0.47 |
| 1:GD:402:ALA:N | 1:GD:403:PRO:HD2 | 2.29 | 0.47 |
| 1:GE:514:THR:HG22 | 1:GE:539:ARG:HB2 | 1.96 | 0.47 |
| 1:GE:649:GLN:N | 1:GE:649:GLN:OE1 | 2.32 | 0.47 |
| 2:GF:366:TYR:HB2 | 2:GF:380:ILE:CD1 | 2.41 | 0.47 |
| 2:GF:555:ARG:HD2 | 2:GF:557:VAL:O | 2.14 | 0.47 |
| 2:GF:840:ARG:NH2 | 2:GF:843:LYS:HG2 | 2.28 | 0.47 |
| 3:GG:47:TRP:CD1 | 3:GG:48:SER:N | 2.83 | 0.47 |
| 5:HB:316:ILE:HG22 | 5:HB:318:GLN:HG3 | 1.96 | 0.47 |
| 5:HB:486:VAL:HG22 | 5:HD:591:PRO:O | 2.14 | 0.47 |
| 5:HC:170:GLU:O | 5:HC:171:VAL:HG12 | 2.14 | 0.47 |
| 5:HC:2:LYS:H | 5:HD:41:ASP:HB3 | 1.79 | 0.47 |
| 5:HC:321:ALA:HA | 5:HC:358:VAL:HB | 1.95 | 0.47 |
| 5:HC:358:VAL:HG23 | 5:HC:371:PHE:HD1 | 1.80 | 0.47 |
| 5:HB:1:MET:H3 | 5:HC:41:ASP:HB3 | 1.80 | 0.47 |
| 5:HC:30:PHE:HE1 | 5:HD:30:PHE:HE1 | 1.62 | 0.47 |
| 5:HD:362:GLU:HG2 | 5:HD:368:ILE:HG22 | 1.96 | 0.47 |
| 5:HD:358:VAL:HA | 5:HD:371:PHE:HA | 1.96 | 0.47 |
| 5:HD:63:GLU:HB2 | 5:HD:68:TYR:OH | 2.14 | 0.47 |
| 5:HD:96:ARG:NH1 | 5:HD:132:ASP:OD2 | 2.48 | 0.47 |
| 7:HH:323:GLY:HA2 | 7:HI:326:ILE:HG23 | 1.96 | 0.47 |
| 7:HI:77:THR:HG23 | 7:HI:79:ALA:H | 1.77 | 0.47 |
| 7:HJ:266:THR:HG22 | 7:HJ:280:ALA:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HJ:476:ASP:O | 7:HJ:479:ASN:ND2 | 2.47 | 0.47 |
| 7:HJ:63:GLU:OE1 | 7:HJ:80:THR:HA | 2.13 | 0.47 |
| 5:I:10:VAL:HG11 | 5:K:10:VAL:HG21 | 29.87 | 0.47 |
| 5:I:182:ARG:NH1 | 5:J:299:ILE:HG12 | 2.29 | 0.47 |
| 5:J:49:TRP:HZ3 | 5:J:96:ARG:CD | 2.26 | 0.47 |
| 6:M:10:VAL:CA | 6:N:13:ARG:HD2 | 2.31 | 0.47 |
| 6:N:76:GLY:HA2 | 6:N:215:PHE:HZ | 1.79 | 0.47 |
| 7:O:329:ASN:CG | 7:Q:333:THR:HB | 2.34 | 0.47 |
| 7:Q:31:ASP:CG | 7:Q:34:ALA:H | 2.17 | 0.47 |
| 8:R:118:ARG:HE | 8:S:62:GLY:HA2 | 1.80 | 0.47 |
| 8:S:85:PHE:HB3 | 8:S:137:VAL:HG21 | 1.96 | 0.47 |
| 12:W:110:LEU:HG | 12:W:177:TRP:HD1 | 1.79 | 0.47 |
| 1:Y:194:ARG:HA | 1:Y:197:VAL:HG23 | 1.97 | 0.47 |
| 13:YA:121[E]:TYR:OH | 13:YA:123[E]:ARG:NH2 | 2.48 | 0.47 |
| 13:YA:370[C]:ASN:ND2 | 13:YA:372[C]:SER:HB3 | 2.29 | 0.47 |
| 13:YA:447[D]:ASN:HB3 | 13:YC:376[D]:PHE:CE2 | 2.49 | 0.47 |
| 13:YA:447[F]:ASN:HB3 | 13:YC:376[F]:PHE:CE2 | 2.49 | 0.47 |
| 13:YA:67[F]:SER:HB3 | 13:YB:123[F]:ARG:HB2 | 1.95 | 0.47 |
| 13:YB:158[A]:PRO:HB2 | 13:YC:473[A]:GLN:OE1 | 2.14 | 0.47 |
| 13:YB:189[F]:LYS:HA | 13:YB:234[F]:GLY:O | 2.14 | 0.47 |
| 13:YA:571[C]:ARG:HD3 | 13:YB:564[C]:GLN:HE22 | 1.79 | 0.47 |
| 13:YB:69[D]:ILE:HG12 | 13:YC:396[D]:GLU:HA | 1.96 | 0.47 |
| 13:YC:12[A]:VAL:HG21 | 14:YE:256[A]:HIS:CE1 | 2.49 | 0.47 |
| 13:YC:12[E]:VAL:HG21 | 14:YE:256[E]:HIS:CE1 | 2.48 | 0.47 |
| 13:YC:189[A]:LYS:HA | 13:YC:234[A]:GLY:O | 2.14 | 0.47 |
| 13:YC:24[C]:LEU:HD23 | 14:YF:259[C]:LEU:CD2 | 2.44 | 0.47 |
| 13:YA:452[D]:GLY:CA | 13:YC:321[D]:LYS:HD3 | 2.40 | 0.47 |
| 13:YC:370[D]:ASN:ND2 | 13:YC:372[D]:SER:HB3 | 2.29 | 0.47 |
| 13:YC:379[F]:PRO:HG2 | 13:YC:429[F]:ARG:NE | 2.29 | 0.47 |
| 13:YC:76[B]:PRO:HB2 | 13:YC:98[B]:GLY:CA | 2.44 | 0.47 |
| 14:YD:14[D]:VAL:HG11 | 14:YD:52[D]:LEU:HD11 | 1.96 | 0.47 |
| 14:YD:185[D]:PHE:CD2 | 14:YD:297[D]:ARG:HA | 2.49 | 0.47 |
| 14:YD:254[C]:TYR:CD2 | 14:YD:265[C]:MET:HG2 | 2.49 | 0.47 |
| 14:YD:310[A]:CYS:SG | 14:YD:355[A]:LEU:HB2 | 2.54 | 0.47 |
| 14:YD:328[D]:ASP:OD1 | 14:YD:329[D]:SER:N | 2.47 | 0.47 |
| 14:YE:185[B]:PHE:CD2 | 14:YE:297[B]:ARG:HA | 2.49 | 0.47 |
| 14:YE:185[C]:PHE:CD2 | 14:YE:297[C]:ARG:HA | 2.49 | 0.47 |
| 14:YE:212[D]:ILE:HG22 | 14:YE:327[D]:ASN:HB2 | 1.96 | 0.47 |
| 14:YE:310[A]:CYS:SG | 14:YE:355[A]:LEU:HB2 | 2.54 | 0.47 |
| 14:YE:47[F]:ARG:O | 14:YE:48[F]:ASN:ND2 | 2.46 | 0.47 |
| 13:YC:34[D]:LEU:HD13 | 14:YF:163[D]:THR:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:V:175:SER:HA | 14:YF:217[C]:SER:HB2 | 1.96 | 0.47 |
| 14:YF:254[E]:TYR:CD2 | 14:YF:265[E]:MET:HG2 | 2.49 | 0.47 |
| 14:YF:304[A]:TYR:HB3 | 14:YF:358[A]:PHE:HD1 | 1.78 | 0.47 |
| 14:YF:310[D]:CYS:SG | 14:YF:355[D]:LEU:HB2 | 2.54 | 0.47 |
| 14:YF:189[D]:TRP:CD1 | 14:YF:320[D]:PRO:HG2 | 2.50 | 0.47 |
| 14:YF:31[A]:LEU:O | 14:YF:35[A]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:54[A]:PHE:CZ | 14:YF:105[A]:ILE:HD11 | 2.48 | 0.47 |
| 2:Z:1025:PRO:C | 2:Z:1027:GLN:H | 2.17 | 0.47 |
| 2:Z:366:TYR:HB2 | 2:Z:380:ILE:CD1 | 2.41 | 0.47 |
| 2:Z:454:ASN:HB2 | 2:Z:471:VAL:HG21 | 1.96 | 0.47 |
| 2:Z:494:GLU:HB2 | 2:Z:498:TRP:HB2 | 1.96 | 0.47 |
| 2:Z:85:ALA:HB2 | 2:Z:91:GLN:HE22 | 1.79 | 0.47 |
| 1:A:112:LEU:HD13 | 1:A:297:VAL:HG12 | 1.96 | 0.47 |
| 1:A:402:ALA:N | 1:A:403:PRO:HD2 | 2.29 | 0.47 |
| 1:A:634:THR:HB | 1:A:638:SER:O | 2.14 | 0.47 |
| 5:AC:110:VAL:HG22 | 5:AC:123:PRO:HB3 | 1.94 | 0.47 |
| 5:AC:180:VAL:HG13 | 5:AC:181:PHE:N | 2.29 | 0.47 |
| 5:AD:400:ILE:HG12 | 5:AE:402:GLU:OE2 | 2.14 | 0.47 |
| 7:AI:195:THR:O | 7:AI:198:GLN:N | 2.48 | 0.47 |
| 7:AI:84:ARG:NH1 | 7:BA:85:LEU:HD22 | 2.30 | 0.47 |
| 1:BH:378:PRO:HG3 | 1:BH:384:LEU:HG | 1.95 | 0.47 |
| 1:BI:129:THR:HG22 | 1:BI:147:SER:HB3 | 1.96 | 0.47 |
| 2:BJ:229:VAL:O | 2:BJ:249:GLY:HA2 | 2.14 | 0.47 |
| 2:BJ:520:SER:O | 2:BJ:522:THR:HG23 | 2.14 | 0.47 |
| 3:CA:147:LEU:HD23 | 3:CA:149:ASP:N | 2.30 | 0.47 |
| 3:CA:43:ARG:N | 3:CA:74:HIS:HB3 | 2.28 | 0.47 |
| 5:CF:365:ILE:HB | 5:CF:366:PRO:HD2 | 1.96 | 0.47 |
| 5:CG:192:ARG:HB2 | 5:CG:245:GLU:HB2 | 1.95 | 0.47 |
| 5:CG:288:MET:CE | 5:CG:292:PRO:HD3 | 2.44 | 0.47 |
| 5:CG:358:VAL:HA | 5:CG:371:PHE:HA | 1.96 | 0.47 |
| 5:CG:490:TRP:CD1 | 5:CG:516:ALA:HA | 2.49 | 0.47 |
| 5:CH:129:ARG:HG3 | 5:CH:130:PHE:H | 1.80 | 0.47 |
| 5:CH:202:TYR:CZ | 5:CH:225:LEU:HB2 | 2.49 | 0.47 |
| 3:D:57:ALA:HB2 | 3:E:7:ILE:HG12 | 1.97 | 0.47 |
| 7:DD:365:GLY:N | 7:DD:392:LEU:HB2 | 2.29 | 0.47 |
| 3:E:248:ARG:HA | 3:E:331:LEU:HD23 | 1.97 | 0.47 |
| 2:EC:1025:PRO:C | 2:EC:1027:GLN:H | 2.17 | 0.47 |
| 2:EC:182:GLN:N | 2:EC:182:GLN:OE1 | 2.42 | 0.47 |
| 3:ED:131:TYR:CD2 | 3:ED:170:PRO:HG2 | 2.47 | 0.47 |
| 3:ED:47:TRP:CD1 | 3:ED:48:SER:N | 2.83 | 0.47 |
| 3:EE:29:GLY:HA2 | 3:EE:34:LYS:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:186:TYR:HB3 | 5:EI:227:GLY:O | 2.14 | 0.47 |
| 5:EI:217:GLU:HB2 | 5:EI:222:LEU:HB2 | 1.97 | 0.47 |
| 5:EJ:506:LEU:HD23 | 5:EJ:512:PRO:HA | 1.96 | 0.47 |
| 5:EJ:64:TRP:O | 5:EJ:93:ILE:HG22 | 2.14 | 0.47 |
| 5:FA:63:GLU:HB2 | 5:FA:68:TYR:OH | 2.14 | 0.47 |
| 6:FB:47:PHE:CZ | 6:FB:49:GLU:HB2 | 2.49 | 0.47 |
| 5:FA:318:GLN:HB3 | 6:FC:4:LEU:CG | 2.41 | 0.47 |
| 7:FE:367:VAL:O | 7:FE:389:ASN:HA | 2.13 | 0.47 |
| 7:FE:263:VAL:O | 7:FF:260:ARG:HA | 2.14 | 0.47 |
| 7:FE:289:GLN:HB2 | 7:FF:286:ASP:O | 2.13 | 0.47 |
| 7:FG:266:THR:HG22 | 7:FG:280:ALA:O | 2.13 | 0.47 |
| 8:FH:31:ASN:OD1 | 8:FH:32:PHE:N | 2.48 | 0.47 |
| 4:G:200:ALA:HB3 | 4:G:221:ILE:HD11 | 1.96 | 0.47 |
| 11:GB:14:LYS:HE2 | 11:GB:19:ASN:HA | 1.96 | 0.47 |
| 12:GC:214:VAL:HG23 | 12:GC:249:GLN:O | 2.15 | 0.47 |
| 1:GD:508:ARG:HH22 | 1:GD:577:PHE:CA | 2.27 | 0.47 |
| 1:GE:205:GLU:O | 1:GE:206:TRP:HD1 | 1.98 | 0.47 |
| 2:GF:213:ASN:HB2 | 2:GF:289:PHE:CE1 | 2.50 | 0.47 |
| 3:GG:7:ILE:HD11 | 3:GH:316:PRO:HG2 | 1.95 | 0.47 |
| 3:GG:233:GLN:HB2 | 3:GH:289:ASN:HD21 | 1.79 | 0.47 |
| 4:GI:50:VAL:C | 4:GI:52:ASN:H | 2.17 | 0.47 |
| 4:GJ:114:GLY:HA3 | 4:GJ:143:TYR:CE2 | 2.49 | 0.47 |
| 5:HB:139:ALA:O | 5:HB:141:GLY:N | 2.47 | 0.47 |
| 5:HB:217:GLU:HB2 | 5:HB:222:LEU:HB2 | 1.97 | 0.47 |
| 5:HB:262:GLN:OE1 | 5:HD:319:GLU:HG3 | 2.15 | 0.47 |
| 5:HC:132:ASP:N | 5:HC:149:LYS:O | 2.47 | 0.47 |
| 5:HC:507:ASP:OD2 | 5:HC:511:ASN:HB2 | 2.14 | 0.47 |
| 5:HC:542:LEU:HD11 | 5:HD:569:TYR:HE2 | 1.79 | 0.47 |
| 5:HD:339:GLU:HG3 | 5:HD:340:VAL:HG13 | 1.97 | 0.47 |
| 6:HF:127:ALA:HA | 6:HF:130:ARG:HH11 | 1.79 | 0.47 |
| 6:HE:54:SER:O | 6:HF:164:GLN:NE2 | 2.46 | 0.47 |
| 6:HG:125:PHE:O | 6:HG:129:VAL:HG23 | 2.14 | 0.47 |
| 7:HH:468:PHE:HB2 | 7:HJ:479:ASN:O | 2.15 | 0.47 |
| 7:HH:84:ARG:NH1 | 7:HJ:85:LEU:HD22 | 2.30 | 0.47 |
| 5:I:258:TYR:OH | 5:I:260:ARG:HB2 | 2.14 | 0.47 |
| 5:I:339:GLU:HG3 | 5:I:340:VAL:HG13 | 1.96 | 0.47 |
| 5:J:103:ASN:CG | 5:J:104:VAL:H | 2.17 | 0.47 |
| 5:J:289:LYS:HD2 | 5:J:372:ASP:HB3 | 1.95 | 0.47 |
| 5:K:362:GLU:HG2 | 5:K:368:ILE:HG22 | 1.97 | 0.47 |
| 5:K:372:ASP:N | 5:K:372:ASP:OD1 | 2.48 | 0.47 |
| 6:N:127:ALA:HA | 6:N:130:ARG:HH11 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:N:125:PHE:O | 6:N:129:VAL:HG23 | 2.14 | 0.47 |
| 7:O:173:ILE:HD11 | 7:Q:174:ALA:HB2 | 1.96 | 0.47 |
| 7:P:368:SER:HA | 7:P:389:ASN:HD22 | 1.79 | 0.47 |
| 7:Q:142:ILE:HG22 | 7:Q:143:LYS:N | 2.29 | 0.47 |
| 7:Q:456:ASP:HA | 7:Q:462:ASN:HD21 | 1.79 | 0.47 |
| 8:S:112:ILE:HD11 | 8:S:126:GLU:OE2 | 2.15 | 0.47 |
| 1:X:402:ALA:N | 1:X:403:PRO:HD2 | 2.29 | 0.47 |
| 13:YA:121[B]:TYR:OH | 13:YA:123[B]:ARG:NH2 | 2.48 | 0.47 |
| 13:YA:12[C]:VAL:HG21 | 14:YF:256[C]:HIS:CE1 | 2.48 | 0.47 |
| 13:YA:16[C]:GLU:CD | 13:YA:30[C]:ARG:HH11 | 2.17 | 0.47 |
| 13:YA:379[A]:PRO:HG2 | 13:YA:429[A]:ARG:NE | 2.30 | 0.47 |
| 13:YA:379[D]:PRO:HG2 | 13:YA:429[D]:ARG:NE | 2.30 | 0.47 |
| 13:YA:453[E]:ASP:OD1 | 13:YC:321[E]:LYS:HG2 | 2.14 | 0.47 |
| 13:YA:565[A]:TYR:O | 13:YC:572[A]:ILE:HA | 2.14 | 0.47 |
| 13:YA:567[A]:ILE:HG23 | 13:YB:565[A]:TYR:CE2 | 2.49 | 0.47 |
| 13:YA:76[B]:PRO:HB2 | 13:YA:98[B]:GLY:CA | 2.44 | 0.47 |
| 13:YB:379[C]:PRO:HG2 | 13:YB:429[C]:ARG:NE | 2.29 | 0.47 |
| 13:YB:379[F]:PRO:HG2 | 13:YB:429[F]:ARG:NE | 2.29 | 0.47 |
| 13:YA:567[F]:ILE:HG23 | 13:YB:565[F]:TYR:CE2 | 2.49 | 0.47 |
| 13:YB:76[B]:PRO:HB2 | 13:YB:98[B]:GLY:CA | 2.44 | 0.47 |
| 13:YC:121[B]:TYR:OH | 13:YC:123[B]:ARG:NH2 | 2.48 | 0.47 |
| 13:YB:546[B]:VAL:HA | 13:YC:538[B]:VAL:O | 2.14 | 0.47 |
| 14:YD:214[E]:GLY:O | 14:YD:215[E]:GLU:HG3 | 2.15 | 0.47 |
| 14:YD:244[B]:LYS:O | 14:YD:247[B]:PRO:HD2 | 2.14 | 0.47 |
| 14:YD:304[E]:TYR:HB3 | 14:YD:358[E]:PHE:HD1 | 1.78 | 0.47 |
| 14:YD:61[F]:HIS:NE2 | 14:YF:332[F]:GLN:HB3 | 2.30 | 0.47 |
| 1:BH:130:ARG:HD3 | 14:YE:181[B]:GLY:HA2 | 1.95 | 0.47 |
| 14:YE:189[C]:TRP:CD1 | 14:YE:320[C]:PRO:HG2 | 2.50 | 0.47 |
| 14:YE:244[F]:LYS:O | 14:YE:247[F]:PRO:HD2 | 2.14 | 0.47 |
| 14:YE:254[A]:TYR:CD2 | 14:YE:265[A]:MET:HG2 | 2.49 | 0.47 |
| 14:YE:31[C]:LEU:O | 14:YE:35[C]:ILE:HG22 | 2.14 | 0.47 |
| 14:YE:72[D]:ILE:O | 14:YE:86[D]:ARG:N | 2.47 | 0.47 |
| 14:YF:310[C]:CYS:SG | 14:YF:355[C]:LEU:HB2 | 2.54 | 0.47 |
| 2:Z:196:GLU:HG2 | 2:Z:197:GLY:N | 2.29 | 0.47 |
| 1:A:145:PHE:HZ | 1:A:286:PHE:CE1 | 2.32 | 0.47 |
| 1:A:525:ASN:HB3 | 1:A:528:THR:HG21 | 1.96 | 0.47 |
| 4:AA:139:VAL:HG13 | 4:AA:164:ILE:HD12 | 1.97 | 0.47 |
| 4:AA:157:THR:O | 4:AA:159:VAL:HG23 | 2.13 | 0.47 |
| 4:AB:85:HIS:HD2 | 4:AB:109:PHE:HE1 | 1.62 | 0.47 |
| 5:AC:97:ASP:HB3 | 5:AC:99:PHE:O | 2.13 | 0.47 |
| 5:AD:166:GLU:OE1 | 5:AD:166:GLU:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:490:TRP:CD1 | 5:AD:516:ALA:HA | 2.49 | 0.47 |
| 5:AD:48:ALA:C | 5:AD:49:TRP:HD1 | 2.17 | 0.47 |
| 5:AE:313:PHE:CE1 | 6:AG:8:ALA:HB1 | 2.47 | 0.47 |
| 7:AI:32:VAL:HA | 7:AI:35:ALA:HB3 | 1.97 | 0.47 |
| 1:B:194:ARG:HA | 1:B:197:VAL:HG23 | 1.97 | 0.47 |
| 1:B:20:ILE:O | 1:B:22:VAL:HG23 | 2.14 | 0.47 |
| 1:B:363:PHE:CG | 1:B:636:ASP:HB2 | 2.50 | 0.47 |
| 7:BA:365:GLY:CA | 7:BA:392:LEU:HB2 | 2.45 | 0.47 |
| 7:BA:456:ASP:HA | 7:BA:462:ASN:HD21 | 1.79 | 0.47 |
| 10:BE:205:LYS:HB2 | 10:BE:311:PHE:CZ | 2.49 | 0.47 |
| 1:BH:518:ASN:HA | 1:BH:535:LEU:HB3 | 1.96 | 0.47 |
| 1:BI:231:ASP:OD1 | 1:BI:232:GLY:N | 2.46 | 0.47 |
| 1:BI:363:PHE:CG | 1:BI:636:ASP:HB2 | 2.50 | 0.47 |
| 1:BI:37:LEU:HD11 | 1:BI:53:LEU:HD21 | 1.97 | 0.47 |
| 2:BJ:406:LEU:CD1 | 2:BJ:413:TRP:HA | 2.44 | 0.47 |
| 1:BH:68:GLN:HA | 2:BJ:682:GLN:NE2 | 2.30 | 0.47 |
| 2:BJ:20:GLN:HG2 | 2:BJ:70:ASP:CG | 2.34 | 0.47 |
| 2:BJ:986:ARG:HH22 | 3:CA:323:ASP:HB2 | 1.80 | 0.47 |
| 2:C:357:ILE:HG23 | 2:C:358:THR:N | 2.30 | 0.47 |
| 2:C:698:GLU:HG3 | 2:C:699:HIS:N | 2.30 | 0.47 |
| 2:C:928:GLU:HA | 2:C:961:VAL:O | 2.14 | 0.47 |
| 3:CA:196:PRO:O | 3:CA:199:SER:HB2 | 2.14 | 0.47 |
| 3:CA:246:THR:HA | 3:CA:332:PHE:O | 2.15 | 0.47 |
| 3:CB:13:THR:HG22 | 3:CB:15:LYS:H | 1.78 | 0.47 |
| 3:CB:193:GLU:HG2 | 3:CB:224:GLY:HA3 | 1.95 | 0.47 |
| 5:CF:194:LYS:HB3 | 5:CF:196:ARG:H | 1.78 | 0.47 |
| 5:CF:217:GLU:HB2 | 5:CF:222:LEU:HB2 | 1.97 | 0.47 |
| 5:CF:339:GLU:HG3 | 5:CF:340:VAL:HG13 | 1.96 | 0.47 |
| 2:BJ:976:SER:HB2 | 5:CG:10:VAL:HG21 | 1.95 | 0.47 |
| 5:CG:170:GLU:O | 5:CG:171:VAL:HG12 | 2.14 | 0.47 |
| 5:CH:314:ASN:ND2 | 6:CJ:8:ALA:O | 2.47 | 0.47 |
| 5:CG:567:THR:O | 5:CH:551:ILE:HA | 2.15 | 0.47 |
| 6:CJ:127:ALA:HA | 6:CJ:130:ARG:HH11 | 1.79 | 0.47 |
| 3:D:47:TRP:CD1 | 3:D:48:SER:N | 2.83 | 0.47 |
| 7:DB:503:ASN:OD1 | 7:DD:446:LYS:N | 2.45 | 0.47 |
| 7:DB:504:ARG:HA | 7:DD:422:LYS:HB3 | 1.97 | 0.47 |
| 7:DB:312:GLY:N | 7:DC:316:THR:O | 2.38 | 0.47 |
| 7:DD:365:GLY:CA | 7:DD:392:LEU:HB2 | 2.45 | 0.47 |
| 7:DC:399:PHE:CD1 | 7:DD:401:ARG:HB3 | 2.50 | 0.47 |
| 3:D:310:ILE:HB | 3:E:16:PHE:HB2 | 1.96 | 0.47 |
| 3:E:232:GLN:OE1 | 2:GF:484:HIS:ND1 | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:47:TRP:CD1 | 3:E:270:ARG:HD2 | 2.50 | 0.47 |
| 3:E:71:MET:HG3 | 3:E:271:GLN:NE2 | 2.29 | 0.47 |
| 1:EA:521:ARG:NH1 | 1:EA:560:SER:O | 2.47 | 0.47 |
| 1:EB:194:ARG:HA | 1:EB:197:VAL:HG23 | 1.97 | 0.47 |
| 1:EB:205:GLU:O | 1:EB:206:TRP:HD1 | 1.97 | 0.47 |
| 2:EC:643:PRO:HG2 | 11:GB:84:TYR:CE2 | 2.48 | 0.47 |
| 3:EE:72:TRP:HZ3 | 3:EE:275:ILE:HD13 | 1.77 | 0.47 |
| 2:EC:898:MET:HE1 | 3:EE:315:ARG:HH12 | 1.79 | 0.47 |
| 4:EH:212:ARG:HG3 | 4:EH:213:LYS:HG3 | 1.96 | 0.47 |
| 5:EJ:10:VAL:HG13 | 5:EJ:13:ASP:HB2 | 1.95 | 0.47 |
| 5:EJ:192:ARG:O | 5:EJ:244:ILE:HA | 2.15 | 0.47 |
| 5:EI:591:PRO:HA | 5:EJ:520:GLY:O | 2.14 | 0.47 |
| 5:FA:202:TYR:CZ | 5:FA:225:LEU:HB2 | 2.49 | 0.47 |
| 7:FE:12:GLU:HG3 | 7:FE:15:TYR:H | 1.80 | 0.47 |
| 7:FF:228:ILE:H | 7:FG:226:GLY:H | 1.62 | 0.47 |
| 7:FF:411:ASN:O | 7:FF:415:ASN:ND2 | 2.48 | 0.47 |
| 7:FG:365:GLY:N | 7:FG:392:LEU:HB2 | 2.29 | 0.47 |
| 7:FE:452:GLY:HA2 | 7:FG:482:TYR:CD2 | 2.49 | 0.47 |
| 4:G:202:LEU:HD21 | 4:G:254:PHE:CZ | 2.50 | 0.47 |
| 12:DJ:153:ARG:HH22 | 12:GC:184:PRO:HA | 1.79 | 0.47 |
| 1:GD:155:ARG:HG2 | 1:GD:156:ASP:O | 2.14 | 0.47 |
| 1:GD:210:THR:HG22 | 1:GD:226:MET:H | 1.79 | 0.47 |
| 1:GD:252:LEU:O | 1:GD:252:LEU:HD12 | 2.15 | 0.47 |
| 1:GD:5:PRO:HG3 | 1:GD:36:TRP:CZ2 | 2.49 | 0.47 |
| 4:GJ:194:ARG:HE | 4:GJ:259:ASN:HA | 1.78 | 0.47 |
| 4:GJ:53:GLY:HA3 | 4:HA:7:LYS:HE2 | 1.96 | 0.47 |
| 4:HA:50:VAL:C | 4:HA:52:ASN:H | 2.17 | 0.47 |
| 4:HA:85:HIS:HD2 | 4:HA:109:PHE:HE1 | 1.62 | 0.47 |
| 5:HB:365:ILE:HB | 5:HB:366:PRO:HD2 | 1.96 | 0.47 |
| 5:HB:535:THR:O | 5:HD:576:THR:N | 2.34 | 0.47 |
| 5:HC:359:GLU:H | 5:HC:370:HIS:C | 2.16 | 0.47 |
| 5:HD:164:ARG:HA | 5:HD:181:PHE:HZ | 1.79 | 0.47 |
| 5:HD:186:TYR:HE1 | 5:HD:246:THR:HA | 1.78 | 0.47 |
| 5:HD:358:VAL:HG23 | 5:HD:371:PHE:HD1 | 1.78 | 0.47 |
| 6:HE:76:GLY:HA2 | 6:HE:215:PHE:HZ | 1.80 | 0.47 |
| 7:HI:516:ASN:ND2 | 7:HJ:401:ARG:HD2 | 2.30 | 0.47 |
| 5:I:180:VAL:HG13 | 5:I:181:PHE:N | 2.29 | 0.47 |
| 5:I:423:THR:O | 7:BA:495:GLN:NE2 | 2.31 | 0.47 |
| 8:IA:112:ILE:HD11 | 8:IA:126:GLU:OE2 | 2.15 | 0.47 |
| 11:IE:182:ASN:ND2 | 14:YF:327[B]:ASN:HD22 | 2.12 | 0.47 |
| 5:I:317:LEU:HD13 | 5:J:312:ARG:NH2 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:290:SER:CB | 5:J:371:PHE:H | 2.27 | 0.47 |
| 5:J:477:SER:HB2 | 5:J:602:ALA:HB3 | 1.96 | 0.47 |
| 5:K:96:ARG:NH1 | 5:K:132:ASP:OD2 | 2.48 | 0.47 |
| 5:K:339:GLU:HG3 | 5:K:340:VAL:HG13 | 1.97 | 0.47 |
| 5:K:39:ASP:HB2 | 5:K:44:TYR:CE2 | 2.48 | 0.47 |
| 6:L:76:GLY:HA2 | 6:L:215:PHE:HZ | 1.79 | 0.47 |
| 8:S:140:LEU:HD23 | 8:IB:41:LEU:HD22 | 1.97 | 0.47 |
| 1:X:5:PRO:HG3 | 1:X:36:TRP:CZ2 | 2.49 | 0.47 |
| 13:YA:461[B]:SER:HA | 13:YC:468[B]:ASP:HB3 | 1.96 | 0.47 |
| 13:YA:470[E]:ARG:HD2 | 13:YC:474[E]:ILE:HD11 | 1.97 | 0.47 |
| 13:YB:81[C]:ARG:HB3 | 13:YB:100[C]:TYR:CZ | 2.50 | 0.47 |
| 13:YB:116[C]:ASP:OD2 | 13:YB:121[C]:TYR:N | 2.43 | 0.47 |
| 13:YB:379[D]:PRO:HG2 | 13:YB:429[D]:ARG:NE | 2.30 | 0.47 |
| 13:YB:44[A]:VAL:HG11 | 14:YD:272[A]:GLU:HB3 | 1.96 | 0.47 |
| 13:YC:121[E]:TYR:OH | 13:YC:123[E]:ARG:NH2 | 2.48 | 0.47 |
| 13:YC:370[B]:ASN:ND2 | 13:YC:372[B]:SER:HB3 | 2.30 | 0.47 |
| 13:YC:379[E]:PRO:HG2 | 13:YC:429[E]:ARG:NE | 2.29 | 0.47 |
| 13:YA:461[F]:SER:HA | 13:YC:468[F]:ASP:HB3 | 1.96 | 0.47 |
| 14:YD:189[B]:TRP:CD1 | 14:YD:320[B]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:244[C]:LYS:O | 14:YD:247[C]:PRO:HD2 | 2.14 | 0.47 |
| 14:YD:31[B]:LEU:O | 14:YD:35[B]:ILE:HG22 | 2.14 | 0.47 |
| 14:YD:54[D]:PHE:CZ | 14:YD:105[D]:ILE:HD11 | 2.49 | 0.47 |
| 14:YE:254[D]:TYR:CD2 | 14:YE:265[D]:MET:HG2 | 2.49 | 0.47 |
| 1:X:287:SER:HB2 | 14:YE:373[F]:LYS:HD2 | 1.96 | 0.47 |
| 14:YF:214[B]:GLY:O | 14:YF:215[B]:GLU:HG3 | 2.14 | 0.47 |
| 14:YF:244[D]:LYS:O | 14:YF:247[D]:PRO:HD2 | 2.14 | 0.47 |
| 13:YC:24[A]:LEU:HD23 | 14:YF:259[A]:LEU:CD2 | 2.45 | 0.47 |
| 14:YF:252[A]:THR:OG1 | 14:YF:271[A]:GLY:O | 2.32 | 0.47 |
| 14:YF:336[F]:GLU:O | 14:YF:359[F]:THR:OG1 | 2.33 | 0.47 |
| 14:YE:236[F]:TRP:N | 14:YF:95[F]:VAL:O | 2.48 | 0.47 |
| 2:Z:357:ILE:HG23 | 2:Z:358:THR:N | 2.30 | 0.47 |
| 2:Z:415:ARG:HH22 | 2:Z:424:ARG:NH1 | 2.11 | 0.47 |
| 15:ZA:66[A]:LYS:O | 15:ZA:68[A]:TYR:CD1 | 2.68 | 0.47 |
| 15:ZA:66[B]:LYS:O | 15:ZA:68[B]:TYR:CD1 | 2.68 | 0.47 |
| 4:AB:202:LEU:HD21 | 4:AB:254:PHE:CZ | 2.50 | 0.47 |
| 5:AC:170:GLU:O | 5:AC:172:GLN:N | 2.48 | 0.47 |
| 5:AC:186:TYR:HE1 | 5:AC:246:THR:HA | 1.80 | 0.47 |
| 5:AC:194:LYS:HB3 | 5:AC:196:ARG:H | 1.78 | 0.47 |
| 5:AD:169:VAL:O | 5:AD:238:ILE:HA | 2.15 | 0.47 |
| 5:AD:163:ALA:HB3 | 5:AD:246:THR:HG22 | 1.96 | 0.47 |
| 5:AD:304:ILE:HG21 | 5:AD:309:LEU:HD12 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:352:SER:HB2 | 5:AD:354:THR:O | 2.14 | 0.47 |
| 5:AE:129:ARG:HG3 | 5:AE:130:PHE:H | 1.80 | 0.47 |
| 5:AE:136:VAL:O | 5:AE:143:TRP:HA | 2.14 | 0.47 |
| 5:AE:164:ARG:HA | 5:AE:181:PHE:CZ | 2.49 | 0.47 |
| 5:AD:567:THR:O | 5:AE:551:ILE:HA | 2.15 | 0.47 |
| 6:AG:69:THR:HA | 6:AH:73:ASN:CB | 2.44 | 0.47 |
| 7:AI:130:GLU:OE2 | 7:AJ:132:ARG:NH1 | 2.38 | 0.47 |
| 7:AI:160:MET:HG3 | 7:AI:164:LYS:HZ1 | 1.78 | 0.47 |
| 7:AJ:142:ILE:HG22 | 7:AJ:143:LYS:O | 2.14 | 0.47 |
| 7:AJ:516:ASN:ND2 | 7:BA:401:ARG:HD2 | 2.29 | 0.47 |
| 1:B:205:GLU:O | 1:B:206:TRP:HD1 | 1.98 | 0.47 |
| 1:B:118:LEU:HG | 1:B:294:ASN:CG | 2.35 | 0.47 |
| 7:BA:73:THR:HG23 | 7:BA:74:LYS:H | 1.78 | 0.47 |
| 10:BE:334:ILE:HG13 | 10:BE:335:ALA:N | 2.30 | 0.47 |
| 1:BH:571:PRO:HA | 1:BH:589:TYR:O | 2.15 | 0.47 |
| 1:BI:41:ASN:OD1 | 1:BI:42:GLU:N | 2.37 | 0.47 |
| 1:BI:485:VAL:HG11 | 1:BI:650:TYR:HE1 | 1.79 | 0.47 |
| 2:BJ:1025:PRO:C | 2:BJ:1027:GLN:H | 2.17 | 0.47 |
| 2:BJ:234:SER:OG | 2:BJ:366:TYR:O | 2.25 | 0.47 |
| 2:BJ:696:ARG:HH12 | 2:BJ:726:PHE:HD1 | 1.63 | 0.47 |
| 2:BJ:712:ASN:HA | 2:BJ:751:LEU:HG | 1.97 | 0.47 |
| 2:BJ:777:LEU:HD12 | 2:BJ:778:THR:H | 1.79 | 0.47 |
| 2:C:91:GLN:HE21 | 2:C:92:SER:H | 1.62 | 0.47 |
| 2:BJ:912:ILE:HD11 | 3:CA:329:ASN:HD22 | 1.79 | 0.47 |
| 3:CA:47:TRP:CD1 | 3:CA:48:SER:N | 2.83 | 0.47 |
| 3:CB:29:GLY:HA2 | 3:CB:34:LYS:HE3 | 1.97 | 0.47 |
| 3:CB:47:TRP:CD1 | 3:CB:270:ARG:HD2 | 2.50 | 0.47 |
| 4:CE:194:ARG:HE | 4:CE:259:ASN:HA | 1.78 | 0.47 |
| 5:CF:354:THR:HG22 | 5:CF:372:ASP:CG | 2.34 | 0.47 |
| 5:CG:163:ALA:HB3 | 5:CG:246:THR:HG22 | 1.96 | 0.47 |
| 5:CG:213:GLY:CA | 5:CG:221:GLU:HB2 | 2.45 | 0.47 |
| 5:CG:526:THR:HG21 | 5:CG:582:PRO:HB2 | 1.97 | 0.47 |
| 5:CH:110:VAL:HG22 | 5:CH:123:PRO:HB3 | 1.97 | 0.47 |
| 5:CH:313:PHE:CE1 | 6:CJ:8:ALA:HB1 | 2.48 | 0.47 |
| 7:DB:342:PRO:HG2 | 7:DB:345:ALA:HB2 | 1.96 | 0.47 |
| 7:DB:359:TRP:NE1 | 7:DC:340:THR:O | 2.29 | 0.47 |
| 11:DI:178:ASN:H | 14:YD:217[D]:SER:C | 2.16 | 0.47 |
| 11:DI:14:LYS:HE2 | 11:DI:19:ASN:HA | 1.96 | 0.47 |
| 2:EC:543:LYS:HE2 | 2:EC:574:LYS:O | 2.14 | 0.47 |
| 2:EC:646:ARG:CD | 2:EC:673:GLN:HE22 | 2.13 | 0.47 |
| 2:EC:808:GLN:HE21 | 2:EC:839:ILE:HG13 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:225:TYR:HE2 | 3:ED:231:TRP:HB3 | 1.79 | 0.47 |
| 4:EF:139:VAL:HG13 | 4:EF:164:ILE:HD12 | 1.97 | 0.47 |
| 4:EH:114:GLY:HA3 | 4:EH:143:TYR:CE2 | 2.49 | 0.47 |
| 5:EI:170:GLU:O | 5:EI:172:GLN:N | 2.48 | 0.47 |
| 5:EI:486:VAL:HG22 | 5:FA:591:PRO:O | 2.13 | 0.47 |
| 5:EJ:116:THR:HA | 5:EJ:121:ALA:HB2 | 1.96 | 0.47 |
| 4:F:200:ALA:HB3 | 4:F:221:ILE:HD11 | 1.96 | 0.47 |
| 5:EJ:590:GLN:OE1 | 5:FA:589:ILE:HA | 2.14 | 0.47 |
| 6:FB:76:GLY:HA2 | 6:FB:215:PHE:HZ | 1.79 | 0.47 |
| 7:FF:99:ARG:HG2 | 7:FF:100:TYR:N | 2.29 | 0.47 |
| 7:FF:415:ASN:O | 7:FF:424:ARG:HD2 | 2.15 | 0.47 |
| 7:FE:95:TYR:HA | 7:FG:98:THR:O | 2.14 | 0.47 |
| 12:GC:187:GLY:O | 12:GC:188:LEU:HD12 | 2.14 | 0.47 |
| 1:GE:179:TYR:CD1 | 1:GE:185:ILE:HD11 | 2.49 | 0.47 |
| 1:GE:179:TYR:HD1 | 1:GE:185:ILE:HD11 | 1.79 | 0.47 |
| 1:GE:194:ARG:HA | 1:GE:197:VAL:HG23 | 1.97 | 0.47 |
| 2:GF:696:ARG:HH12 | 2:GF:726:PHE:HD1 | 1.63 | 0.47 |
| 2:GF:784:GLN:HG2 | 2:GF:830:ARG:HG2 | 1.96 | 0.47 |
| 2:GF:853:ASP:OD1 | 2:GF:854:TYR:N | 2.47 | 0.47 |
| 3:GH:221:THR:O | 3:GH:224:GLY:N | 2.37 | 0.47 |
| 4:GI:85:HIS:HD2 | 4:GI:109:PHE:HE1 | 1.62 | 0.47 |
| 4:H:202:LEU:HD21 | 4:H:254:PHE:CZ | 2.50 | 0.47 |
| 5:HB:180:VAL:HG13 | 5:HB:181:PHE:N | 2.29 | 0.47 |
| 5:HB:259:THR:OG1 | 5:HB:385:TRP:HB2 | 2.14 | 0.47 |
| 5:HC:526:THR:HG21 | 5:HC:582:PRO:HB2 | 1.97 | 0.47 |
| 5:HD:129:ARG:HG3 | 5:HD:130:PHE:H | 1.80 | 0.47 |
| 5:HC:319:GLU:HG3 | 5:HD:262:GLN:OE1 | 2.14 | 0.47 |
| 6:HE:168:LEU:HB2 | 6:HE:180:GLN:OE1 | 2.15 | 0.47 |
| 6:HF:54:SER:HA | 6:HG:164:GLN:HE22 | 1.80 | 0.47 |
| 7:HH:493:GLU:HG3 | 7:HH:496:ARG:HH21 | 1.80 | 0.47 |
| 7:HI:415:ASN:O | 7:HI:424:ARG:HD2 | 2.15 | 0.47 |
| 7:HJ:383:TYR:CE1 | 7:HJ:393:PRO:HG3 | 2.50 | 0.47 |
| 7:HJ:456:ASP:HA | 7:HJ:462:ASN:HD21 | 1.79 | 0.47 |
| 7:HI:429:CYS:SG | 7:HJ:515:TRP:NE1 | 2.86 | 0.47 |
| 2:GF:645:LEU:HD11 | 11:IE:83:TYR:CD1 | 2.50 | 0.47 |
| 5:J:132:ASP:N | 5:J:149:LYS:O | 2.47 | 0.47 |
| 5:I:182:ARG:HH22 | 5:J:299:ILE:HG21 | 1.79 | 0.47 |
| 5:K:129:ARG:HG3 | 5:K:130:PHE:H | 1.80 | 0.47 |
| 5:K:86:VAL:HG13 | 5:K:87:ASN:N | 2.29 | 0.47 |
| 7:P:175:GLN:O | 6:HF:205:ASN:HB2 | 2.15 | 0.47 |
| 7:O:473:LYS:CD | 7:Q:473:LYS:HB3 | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Q:8:HIS:ND1 | 7:Q:8:HIS:O | 2.46 | 0.47 |
| 8:R:10:PHE:CE2 | 8:R:15:PHE:CE1 | 3.01 | 0.47 |
| 8:S:79:HIS:CE1 | 8:S:151:GLN:HE22 | 2.33 | 0.47 |
| 1:X:69:GLN:CD | 1:Y:21:PHE:HZ | 2.18 | 0.47 |
| 1:Y:209:TRP:NE1 | 1:Y:223:ILE:HG12 | 2.30 | 0.47 |
| 1:Y:363:PHE:CG | 1:Y:636:ASP:HB2 | 2.50 | 0.47 |
| 13:YA:81[C]:ARG:HB3 | 13:YA:100[C]:TYR:CZ | 2.50 | 0.47 |
| 13:YA:257[F]:LYS:HE2 | 13:YA:266[F]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YA:307[E]:ALA:HB1 | 13:YA:331[E]:ILE:HD11 | 1.95 | 0.47 |
| 13:YA:387[F]:TYR:CE1 | 13:YA:388[F]:PRO:HB3 | 2.49 | 0.47 |
| 13:YA:464[B]:TYR:OH | 13:YC:454[B]:LYS:NZ | 2.48 | 0.47 |
| 13:YA:470[C]:ARG:HD2 | 13:YC:474[C]:ILE:HD11 | 1.97 | 0.47 |
| 13:YB:147[D]:ILE:O | 13:YB:151[D]:ASN:ND2 | 2.48 | 0.47 |
| 13:YB:147[A]:ILE:O | 13:YB:151[A]:ASN:ND2 | 2.48 | 0.47 |
| 13:YB:189[C]:LYS:HA | 13:YB:234[C]:GLY:O | 2.14 | 0.47 |
| 13:YA:315[B]:LEU:HD23 | 13:YB:367[B]:PRO:HA | 1.95 | 0.47 |
| 13:YB:387[C]:TYR:CE1 | 13:YB:388[C]:PRO:HB3 | 2.49 | 0.47 |
| 13:YA:571[B]:ARG:HD3 | 13:YB:564[B]:GLN:HE22 | 1.80 | 0.47 |
| 13:YB:69[A]:ILE:HG12 | 13:YC:396[A]:GLU:HA | 1.96 | 0.47 |
| 13:YC:379[D]:PRO:HG2 | 13:YC:429[D]:ARG:NE | 2.30 | 0.47 |
| 13:YC:39[F]:ARG:NH1 | 13:YC:113[F]:GLY:HA2 | 2.30 | 0.47 |
| 13:YB:492[D]:GLY:HA3 | 13:YC:485[D]:ASP:HA | 1.97 | 0.47 |
| 13:YA:565[E]:TYR:O | 13:YC:572[E]:ILE:HA | 2.13 | 0.47 |
| 13:YA:34[E]:LEU:HD13 | 14:YD:163[E]:THR:HG21 | 1.96 | 0.47 |
| 14:YD:189[D]:TRP:CD1 | 14:YD:320[D]:PRO:HG2 | 2.50 | 0.47 |
| 11:DI:178:ASN:HB3 | 14:YD:217[D]:SER:H | 1.80 | 0.47 |
| 14:YD:254[F]:TYR:CD2 | 14:YD:265[F]:MET:HG2 | 2.49 | 0.47 |
| 14:YD:310[C]:CYS:SG | 14:YD:355[C]:LEU:HB2 | 2.54 | 0.47 |
| 14:YD:310[D]:CYS:SG | 14:YD:355[D]:LEU:HB2 | 2.54 | 0.47 |
| 14:YD:336[D]:GLU:O | 14:YD:359[D]:THR:OG1 | 2.33 | 0.47 |
| 14:YD:72[D]:ILE:O | 14:YD:86[D]:ARG:N | 2.47 | 0.47 |
| 14:YE:189[D]:TRP:CD1 | 14:YE:320[D]:PRO:HG2 | 2.50 | 0.47 |
| 14:YE:244[A]:LYS:O | 14:YE:247[A]:PRO:HD2 | 2.14 | 0.47 |
| 14:YE:252[C]:THR:OG1 | 14:YE:271[C]:GLY:O | 2.32 | 0.47 |
| 14:YE:310[E]:CYS:SG | 14:YE:355[E]:LEU:HB2 | 2.54 | 0.47 |
| 14:YE:328[C]:ASP:OD1 | 14:YE:329[C]:SER:N | 2.47 | 0.47 |
| 14:YE:54[D]:PHE:CZ | 14:YE:105[D]:ILE:HD11 | 2.49 | 0.47 |
| 14:YF:189[A]:TRP:CD1 | 14:YF:320[A]:PRO:HG2 | 2.50 | 0.47 |
| 14:YF:189[C]:TRP:CD1 | 14:YF:320[C]:PRO:HG2 | 2.50 | 0.47 |
| 14:YF:254[B]:TYR:CD2 | 14:YF:265[B]:MET:HG2 | 2.49 | 0.47 |
| 14:YF:310[E]:CYS:SG | 14:YF:355[E]:LEU:HB2 | 2.54 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:31[D]:LEU:O | 14:YF:35[D]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:328[A]:ASP:OD1 | 14:YF:329[A]:SER:N | 2.47 | 0.47 |
| 14:YF:10[D]:PRO:HD2 | 14:YF:349[D]:ASN:O | 2.15 | 0.47 |
| 2:Z:444:SER:HB2 | 2:Z:512:PRO:HG3 | 1.94 | 0.47 |
| 2:Z:698:GLU:HG3 | 2:Z:699:HIS:N | 2.30 | 0.47 |
| 2:Z:774:SER:HB2 | 2:Z:836:GLY:HA3 | 1.96 | 0.47 |
| 2:Z:881:ARG:NH2 | 2:Z:882:PHE:HE1 | 2.13 | 0.47 |
| 15:ZA:66[F]:LYS:O | 15:ZA:68[F]:TYR:CD1 | 2.68 | 0.47 |
| 1:A:518:ASN:OD1 | 1:A:519:SER:N | 2.48 | 0.47 |
| 5:AC:22:GLY:O | 5:AC:26:ILE:N | 2.37 | 0.47 |
| 5:AC:316:ILE:HD13 | 6:AH:7:LYS:HG3 | 1.97 | 0.47 |
| 5:AD:316:ILE:HD13 | 6:AF:7:LYS:HE3 | 1.95 | 0.47 |
| 5:AD:34:TYR:O | 5:AD:38:GLY:N | 2.37 | 0.47 |
| 5:AD:507:ASP:OD2 | 5:AD:511:ASN:HB2 | 2.14 | 0.47 |
| 5:AD:526:THR:HG21 | 5:AD:582:PRO:HB2 | 1.97 | 0.47 |
| 5:AC:241:THR:HG21 | 5:AE:200:LEU:CD1 | 2.42 | 0.47 |
| 6:AG:127:ALA:HA | 6:AG:130:ARG:HH11 | 1.79 | 0.47 |
| 7:AI:329:ASN:HD21 | 7:BA:335:ASN:H | 1.63 | 0.47 |
| 7:AI:339:ARG:NH1 | 7:BA:356:SER:HB2 | 2.29 | 0.47 |
| 7:AI:477:TRP:CZ3 | 7:AJ:469:VAL:HB | 2.49 | 0.47 |
| 7:BA:160:MET:HG2 | 7:BA:165:THR:HB | 1.96 | 0.47 |
| 7:AJ:216:MET:SD | 7:BA:202:GLY:HA3 | 2.55 | 0.47 |
| 7:BA:220:SER:HB2 | 7:BA:228:ILE:HG12 | 1.97 | 0.47 |
| 7:BA:375:TYR:CZ | 7:BA:392:LEU:HD23 | 2.50 | 0.47 |
| 7:BA:476:ASP:O | 7:BA:479:ASN:ND2 | 2.47 | 0.47 |
| 8:BC:79:HIS:CE1 | 8:BC:151:GLN:HE22 | 2.33 | 0.47 |
| 12:BG:158:LEU:HD21 | 12:BG:216:PHE:CE1 | 2.48 | 0.47 |
| 1:BH:472:ASP:C | 1:BH:474:SER:H | 2.18 | 0.47 |
| 1:BI:205:GLU:O | 1:BI:206:TRP:HD1 | 1.97 | 0.47 |
| 1:BI:20:ILE:O | 1:BI:22:VAL:HG23 | 2.14 | 0.47 |
| 1:BI:372:ALA:N | 1:BI:404:ILE:HD11 | 2.30 | 0.47 |
| 2:BJ:516:TRP:CH2 | 2:BJ:521:ASN:HB2 | 2.49 | 0.47 |
| 2:C:196:GLU:HG2 | 2:C:197:GLY:N | 2.29 | 0.47 |
| 2:C:712:ASN:HA | 2:C:751:LEU:HG | 1.97 | 0.47 |
| 4:CD:139:VAL:HG13 | 4:CD:164:ILE:HD12 | 1.97 | 0.47 |
| 4:CD:202:LEU:HD21 | 4:CD:254:PHE:CZ | 2.50 | 0.47 |
| 5:CF:110:VAL:HG22 | 5:CF:123:PRO:HB3 | 1.94 | 0.47 |
| 5:CF:180:VAL:HG13 | 5:CF:181:PHE:N | 2.29 | 0.47 |
| 5:CF:239:GLY:O | 7:DB:2:SER:N | 2.47 | 0.47 |
| 5:CF:316:ILE:HG22 | 5:CF:318:GLN:HG3 | 1.97 | 0.47 |
| 5:CF:402:GLU:HG3 | 5:CF:406:LEU:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:478:TRP:CH2 | 5:CF:600:ARG:HB2 | 2.50 | 0.47 |
| 5:CG:507:ASP:OD2 | 5:CG:511:ASN:HB2 | 2.14 | 0.47 |
| 5:CH:96:ARG:NH1 | 5:CH:132:ASP:OD2 | 2.48 | 0.47 |
| 5:CH:164:ARG:HA | 5:CH:181:PHE:CZ | 2.49 | 0.47 |
| 5:CH:335:ASP:OD1 | 5:CH:335:ASP:N | 2.47 | 0.47 |
| 6:CJ:47:PHE:CZ | 6:CJ:49:GLU:HB2 | 2.49 | 0.47 |
| 7:DB:195:THR:O | 7:DB:198:GLN:N | 2.48 | 0.47 |
| 7:DB:371:ASP:OD1 | 7:DB:526:LYS:NZ | 2.47 | 0.47 |
| 7:DB:39:ILE:HG22 | 7:DD:44:VAL:CG2 | 2.45 | 0.47 |
| 7:DC:368:SER:HA | 7:DC:389:ASN:HD22 | 1.79 | 0.47 |
| 7:DD:476:ASP:O | 7:DD:479:ASN:ND2 | 2.47 | 0.47 |
| 8:BB:41:LEU:HD22 | 8:DE:140:LEU:HD23 | 1.96 | 0.47 |
| 11:DI:38:ARG:HH11 | 11:DI:187:ILE:HD12 | 1.78 | 0.47 |
| 1:EA:155:ARG:HG2 | 1:EA:156:ASP:O | 2.14 | 0.47 |
| 1:EA:645:ASP:OD1 | 1:EA:645:ASP:N | 2.45 | 0.47 |
| 1:EB:76:TYR:CE2 | 11:GB:31:ASN:HA | 2.49 | 0.47 |
| 2:EC:339:ASP:O | 2:EC:341:LEU:N | 2.47 | 0.47 |
| 2:EC:50:PRO:O | 2:EC:54:TYR:HB3 | 2.14 | 0.47 |
| 2:EC:555:ARG:HD2 | 2:EC:557:VAL:O | 2.14 | 0.47 |
| 3:ED:42:GLY:HA2 | 3:ED:76:MET:HG3 | 1.97 | 0.47 |
| 4:EG:200:ALA:HB3 | 4:EG:221:ILE:HD11 | 1.96 | 0.47 |
| 5:EI:259:THR:OG1 | 5:EI:385:TRP:HB2 | 2.14 | 0.47 |
| 5:EJ:321:ALA:HA | 5:EJ:358:VAL:HB | 1.95 | 0.47 |
| 5:EJ:358:VAL:HG23 | 5:EJ:371:PHE:HD1 | 1.80 | 0.47 |
| 7:Q:472:ARG:HE | 5:FA:363:ASN:HD21 | 1.63 | 0.47 |
| 6:FC:47:PHE:CZ | 6:FC:49:GLU:HB2 | 2.49 | 0.47 |
| 7:FE:110:VAL:HG12 | 7:FE:111:ASN:N | 2.30 | 0.47 |
| 7:FE:447:HIS:CD2 | 7:FF:447:HIS:CD2 | 2.99 | 0.47 |
| 7:FF:180:GLU:HG2 | 7:FG:179:SER:OG | 2.14 | 0.47 |
| 7:FG:127:ASN:O | 7:FG:131:THR:HG23 | 2.15 | 0.47 |
| 7:FG:220:SER:OG | 7:FG:226:GLY:O | 2.33 | 0.47 |
| 7:FG:329:ASN:OD1 | 7:FG:330:ARG:N | 2.48 | 0.47 |
| 7:FE:485:ASN:OD1 | 7:FG:448:ALA:N | 2.48 | 0.47 |
| 8:FI:31:ASN:OD1 | 8:FI:32:PHE:N | 2.48 | 0.47 |
| 4:F:205:THR:HG22 | 4:G:284:ILE:HD11 | 1.96 | 0.47 |
| 12:GC:241:VAL:O | 12:GC:241:VAL:HG13 | 2.14 | 0.47 |
| 1:GD:518:ASN:OD1 | 1:GD:519:SER:N | 2.48 | 0.47 |
| 1:GE:45:ASP:C | 1:GE:47:ASP:H | 2.10 | 0.47 |
| 1:GE:37:LEU:HD11 | 1:GE:53:LEU:HD21 | 1.97 | 0.47 |
| 2:GF:151:PHE:CD2 | 2:GF:166:PHE:HE1 | 2.33 | 0.47 |
| 2:GF:177:GLN:HE22 | 2:GF:534:VAL:HG12 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:340:PRO:HA | 2:GF:345:TYR:CD1 | 2.50 | 0.47 |
| 3:GG:246:THR:HA | 3:GG:332:PHE:O | 2.15 | 0.47 |
| 4:H:139:VAL:HG13 | 4:H:164:ILE:HD12 | 1.97 | 0.47 |
| 4:G:173:SER:N | 4:H:166:SER:OG | 2.40 | 0.47 |
| 5:HB:84:GLY:C | 5:HB:86:VAL:H | 2.18 | 0.47 |
| 5:HC:360:THR:HG22 | 5:HC:366:PRO:HG3 | 1.96 | 0.47 |
| 5:HD:139:ALA:HB3 | 5:HD:140:PRO:HD3 | 1.96 | 0.47 |
| 5:HD:164:ARG:HA | 5:HD:181:PHE:CZ | 2.49 | 0.47 |
| 5:HD:372:ASP:OD1 | 5:HD:372:ASP:N | 2.48 | 0.47 |
| 5:HD:396:LYS:O | 5:HD:399:ILE:HG13 | 2.14 | 0.47 |
| 6:HG:168:LEU:HB2 | 6:HG:180:GLN:OE1 | 2.15 | 0.47 |
| 6:HG:76:GLY:HA2 | 6:HG:215:PHE:HZ | 1.79 | 0.47 |
| 7:HJ:253:ARG:O | 7:HJ:262:VAL:HG22 | 2.14 | 0.47 |
| 7:HJ:386:ASN:OD1 | 7:HJ:389:ASN:N | 2.24 | 0.47 |
| 5:I:139:ALA:O | 5:I:141:GLY:N | 2.47 | 0.47 |
| 5:I:170:GLU:O | 5:I:172:GLN:N | 2.48 | 0.47 |
| 5:I:186:TYR:HE1 | 5:I:246:THR:HA | 1.80 | 0.47 |
| 5:I:317:LEU:HD21 | 5:J:260:ARG:NH2 | 2.30 | 0.47 |
| 5:I:402:GLU:HG3 | 5:I:406:LEU:HD11 | 1.96 | 0.47 |
| 8:IA:31:ASN:OD1 | 8:IA:32:PHE:N | 2.48 | 0.47 |
| 8:IB:79:HIS:CE1 | 8:IB:151:GLN:HE22 | 2.33 | 0.47 |
| 10:ID:289:ASN:HB2 | 10:ID:290:PRO:HD2 | 1.95 | 0.47 |
| 1:GE:189:ASP:HA | 11:IE:121:TYR:CE2 | 2.49 | 0.47 |
| 11:IE:132:VAL:HA | 11:IE:147:GLU:HA | 1.97 | 0.47 |
| 12:IF:214:VAL:HG23 | 12:IF:249:GLN:O | 2.15 | 0.47 |
| 5:J:163:ALA:HB3 | 5:J:246:THR:HG22 | 1.96 | 0.47 |
| 5:J:192:ARG:HB2 | 5:J:245:GLU:HB2 | 1.95 | 0.47 |
| 5:J:360:THR:HG22 | 5:J:366:PRO:HG3 | 1.96 | 0.47 |
| 5:J:200:LEU:HD11 | 5:K:241:THR:HG21 | 1.97 | 0.47 |
| 7:O:110:VAL:HG12 | 7:O:111:ASN:N | 2.30 | 0.47 |
| 7:O:154:ALA:HB3 | 7:Q:162:PRO:HG2 | 1.97 | 0.47 |
| 7:O:195:THR:O | 7:O:198:GLN:N | 2.48 | 0.47 |
| 7:O:357:ASP:OD1 | 7:P:339:ARG:NH2 | 2.48 | 0.47 |
| 7:O:482:TYR:OH | 7:P:453:GLU:HB2 | 2.14 | 0.47 |
| 7:Q:220:SER:HB2 | 7:Q:228:ILE:HG12 | 1.97 | 0.47 |
| 7:Q:365:GLY:CA | 7:Q:392:LEU:HB2 | 2.45 | 0.47 |
| 7:Q:365:GLY:N | 7:Q:392:LEU:HB2 | 2.29 | 0.47 |
| 8:S:79:HIS:HE1 | 8:S:151:GLN:HE22 | 1.63 | 0.47 |
| 10:U:142:ARG:O | 10:U:143:PHE:HD1 | 1.96 | 0.47 |
| 10:U:289:ASN:HB2 | 10:U:290:PRO:HD2 | 1.95 | 0.47 |
| 12:W:127:SER:HB3 | 12:W:161:SER:HG | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:224:TYR:HA | 1:X:238:PHE:HB3 | 1.96 | 0.47 |
| 1:Y:129:THR:HG22 | 1:Y:147:SER:HB3 | 1.96 | 0.47 |
| 1:Y:179:TYR:HD1 | 1:Y:185:ILE:HD11 | 1.79 | 0.47 |
| 1:Y:231:ASP:OD1 | 1:Y:232:GLY:N | 2.46 | 0.47 |
| 13:YA:370[B]:ASN:ND2 | 13:YA:372[B]:SER:HB3 | 2.30 | 0.47 |
| 13:YA:571[F]:ARG:HD3 | 13:YB:564[F]:GLN:HE22 | 1.80 | 0.47 |
| 13:YA:70[A]:GLY:O | 13:YB:393[A]:MET:HA | 2.14 | 0.47 |
| 13:YB:257[C]:LYS:HE2 | 13:YB:266[C]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YB:553[A]:LYS:HZ2 | 13:YB:553[A]:LYS:HB2 | 1.80 | 0.47 |
| 13:YB:76[B]:PRO:HB2 | 13:YB:98[B]:GLY:N | 2.29 | 0.47 |
| 13:YA:95[E]:ILE:HD11 | 13:YB:83[E]:TYR:CZ | 2.49 | 0.47 |
| 13:YC:257[A]:LYS:HE2 | 13:YC:266[A]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YC:307[E]:ALA:HB1 | 13:YC:331[E]:ILE:HD11 | 1.95 | 0.47 |
| 13:YA:453[C]:ASP:OD1 | 13:YC:321[C]:LYS:HG2 | 2.14 | 0.47 |
| 13:YC:307[F]:ALA:HB1 | 13:YC:331[F]:ILE:HD11 | 1.96 | 0.47 |
| 13:YC:370[E]:ASN:ND2 | 13:YC:372[E]:SER:HB3 | 2.30 | 0.47 |
| 13:YC:379[A]:PRO:HG2 | 13:YC:429[A]:ARG:NE | 2.30 | 0.47 |
| 13:YB:474[D]:ILE:HD13 | 13:YC:470[D]:ARG:HB2 | 1.96 | 0.47 |
| 13:YA:121[C]:TYR:HB3 | 13:YC:66[C]:MET:SD | 2.55 | 0.47 |
| 13:YA:123[C]:ARG:HB2 | 13:YC:67[C]:SER:HB3 | 1.95 | 0.47 |
| 14:YD:185[A]:PHE:CD2 | 14:YD:297[A]:ARG:HA | 2.49 | 0.47 |
| 14:YD:189[A]:TRP:CD1 | 14:YD:320[A]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:189[E]:TRP:CD1 | 14:YD:320[E]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:214[C]:GLY:O | 14:YD:215[C]:GLU:HG3 | 2.14 | 0.47 |
| 14:YD:214[F]:GLY:O | 14:YD:215[F]:GLU:HG3 | 2.15 | 0.47 |
| 14:YD:212[F]:ILE:HG22 | 14:YD:327[F]:ASN:HB2 | 1.97 | 0.47 |
| 14:YD:328[E]:ASP:OD1 | 14:YD:329[E]:SER:N | 2.47 | 0.47 |
| 14:YD:332[E]:GLN:HB3 | 14:YE:61[E]:HIS:NE2 | 2.29 | 0.47 |
| 14:YD:10[D]:PRO:HD2 | 14:YD:349[D]:ASN:O | 2.15 | 0.47 |
| 14:YD:332[F]:GLN:OE1 | 14:YE:101[F]:GLY:HA2 | 2.14 | 0.47 |
| 14:YE:189[F]:TRP:CD1 | 14:YE:320[F]:PRO:HG2 | 2.50 | 0.47 |
| 14:YE:72[E]:ILE:O | 14:YE:86[E]:ARG:N | 2.47 | 0.47 |
| 14:YF:140[E]:TYR:CD2 | 14:YF:147[E]:THR:HA | 2.50 | 0.47 |
| 14:YF:214[F]:GLY:O | 14:YF:215[F]:GLU:HG3 | 2.14 | 0.47 |
| 14:YF:244[E]:LYS:O | 14:YF:247[E]:PRO:HD2 | 2.14 | 0.47 |
| 14:YF:244[C]:LYS:O | 14:YF:247[C]:PRO:HD2 | 2.14 | 0.47 |
| 14:YF:279[C]:ARG:HA | 14:YF:279[C]:ARG:HD3 | 1.43 | 0.47 |
| 14:YF:336[B]:GLU:O | 14:YF:359[B]:THR:OG1 | 2.33 | 0.47 |
| 1:EA:287:SER:HB2 | 14:YF:373[A]:LYS:HD2 | 1.96 | 0.47 |
| 2:Z:213:ASN:HB2 | 2:Z:289:PHE:CE1 | 2.50 | 0.47 |
| 2:Z:254:PHE:HB3 | 2:Z:294:PHE:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:224:TYR:HA | 1:A:238:PHE:HB3 | 1.96 | 0.47 |
| 4:AA:212:ARG:HG3 | 4:AA:213:LYS:HG3 | 1.96 | 0.47 |
| 5:AD:132:ASP:N | 5:AD:149:LYS:O | 2.47 | 0.47 |
| 5:AD:213:GLY:CA | 5:AD:221:GLU:HB2 | 2.45 | 0.47 |
| 5:AD:321:ALA:HA | 5:AD:358:VAL:HB | 1.95 | 0.47 |
| 5:AD:358:VAL:HA | 5:AD:371:PHE:HA | 1.96 | 0.47 |
| 5:AD:477:SER:HB2 | 5:AD:602:ALA:HB3 | 1.96 | 0.47 |
| 5:AE:358:VAL:HA | 5:AE:371:PHE:HA | 1.96 | 0.47 |
| 5:AE:363:ASN:HD21 | 7:FG:472:ARG:HE | 1.63 | 0.47 |
| 5:AC:399:ILE:HD12 | 5:AE:399:ILE:HG12 | 1.97 | 0.47 |
| 6:AG:125:PHE:O | 6:AG:129:VAL:HG23 | 2.14 | 0.47 |
| 7:AI:191:VAL:C | 7:AJ:188:GLN:HA | 2.34 | 0.47 |
| 7:AJ:146:SER:HA | 7:AJ:164:LYS:HZ2 | 1.78 | 0.47 |
| 7:AI:302:ILE:HD12 | 7:AJ:306:PHE:CZ | 2.50 | 0.47 |
| 7:BA:127:ASN:O | 7:BA:131:THR:HG23 | 2.15 | 0.47 |
| 7:BA:329:ASN:OD1 | 7:BA:330:ARG:N | 2.48 | 0.47 |
| 7:BA:77:THR:HG23 | 7:BA:79:ALA:H | 1.79 | 0.47 |
| 8:BB:112:ILE:HD11 | 8:BB:126:GLU:OE2 | 2.15 | 0.47 |
| 11:BF:38:ARG:HH11 | 11:BF:187:ILE:HD12 | 1.79 | 0.47 |
| 12:BG:21:MET:HB3 | 12:BG:204:HIS:O | 2.15 | 0.47 |
| 1:BH:112:LEU:HD13 | 1:BH:297:VAL:HG12 | 1.96 | 0.47 |
| 1:BH:145:PHE:HZ | 1:BH:286:PHE:CE1 | 2.32 | 0.47 |
| 1:BH:182:LEU:HD12 | 1:BH:182:LEU:O | 2.15 | 0.47 |
| 1:BH:229:THR:OG1 | 1:BH:233:ASN:OD1 | 2.30 | 0.47 |
| 1:BH:448:TYR:CE1 | 1:BH:642:PHE:HB2 | 2.49 | 0.47 |
| 1:BH:596:ASN:OD1 | 1:BH:596:ASN:N | 2.47 | 0.47 |
| 1:BH:634:THR:HB | 1:BH:638:SER:O | 2.14 | 0.47 |
| 1:BI:455:PHE:CD2 | 1:BI:456:ASN:N | 2.83 | 0.47 |
| 1:BI:514:THR:HG22 | 1:BI:539:ARG:HB2 | 1.96 | 0.47 |
| 2:BJ:360:ASN:C | 2:BJ:362:LYS:N | 2.65 | 0.47 |
| 2:BJ:720:ARG:HD2 | 1:EB:430:GLN:NE2 | 2.30 | 0.47 |
| 2:BJ:977:ILE:HD13 | 5:CG:12:ASP:HB3 | 1.96 | 0.47 |
| 2:C:177:GLN:HE22 | 2:C:534:VAL:HG12 | 1.80 | 0.47 |
| 2:C:254:PHE:HB3 | 2:C:294:PHE:HB3 | 1.97 | 0.47 |
| 2:C:664:PHE:O | 2:C:667:PHE:HB3 | 2.15 | 0.47 |
| 3:CA:47:TRP:HZ3 | 3:CA:270:ARG:HD3 | 1.79 | 0.47 |
| 4:CC:178:THR:HA | 4:CC:275:ALA:HA | 1.97 | 0.47 |
| 4:CC:202:LEU:HD21 | 4:CC:254:PHE:CZ | 2.50 | 0.47 |
| 4:CE:178:THR:HA | 4:CE:275:ALA:HA | 1.97 | 0.47 |
| 5:CG:103:ASN:CG | 5:CG:104:VAL:H | 2.17 | 0.47 |
| 5:CG:169:VAL:O | 5:CG:238:ILE:HA | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:248:MET:HE3 | 5:CG:254:TRP:HB2 | 1.97 | 0.47 |
| 5:CH:104:VAL:HG13 | 5:CH:105:ASN:H | 1.80 | 0.47 |
| 5:CH:139:ALA:HB3 | 5:CH:140:PRO:HD3 | 1.96 | 0.47 |
| 5:CH:264:ARG:HH22 | 6:CI:2:SER:N | 2.13 | 0.47 |
| 5:CH:63:GLU:HB2 | 5:CH:68:TYR:OH | 2.14 | 0.47 |
| 5:CH:86:VAL:HG13 | 5:CH:87:ASN:N | 2.29 | 0.47 |
| 3:D:131:TYR:CE1 | 3:D:190:TYR:HD1 | 2.33 | 0.47 |
| 3:D:196:PRO:O | 3:D:199:SER:HB2 | 2.14 | 0.47 |
| 7:DC:415:ASN:O | 7:DC:424:ARG:HD2 | 2.15 | 0.47 |
| 7:DD:134:SER:H | 7:DD:142:ILE:HD11 | 1.78 | 0.47 |
| 7:DD:31:ASP:CG | 7:DD:34:ALA:H | 2.18 | 0.47 |
| 11:DI:74:LEU:HD11 | 11:DI:79:ASN:HD21 | 1.79 | 0.47 |
| 12:DJ:110:LEU:HG | 12:DJ:177:TRP:HD1 | 1.79 | 0.47 |
| 12:DJ:21:MET:HB3 | 12:DJ:204:HIS:O | 2.15 | 0.47 |
| 1:EA:252:LEU:O | 1:EA:252:LEU:HD12 | 2.15 | 0.47 |
| 1:EA:46:TYR:HE1 | 9:FJ:17:MET:HB2 | 1.79 | 0.47 |
| 1:EB:37:LEU:HD11 | 1:EB:53:LEU:HD21 | 1.97 | 0.47 |
| 1:EB:514:THR:HG22 | 1:EB:539:ARG:HB2 | 1.96 | 0.47 |
| 2:EC:454:ASN:HB2 | 2:EC:471:VAL:HG21 | 1.96 | 0.47 |
| 2:EC:928:GLU:HA | 2:EC:961:VAL:O | 2.14 | 0.47 |
| 4:EG:202:LEU:HD21 | 4:EG:254:PHE:CZ | 2.50 | 0.47 |
| 4:EH:139:VAL:HG13 | 4:EH:164:ILE:HD12 | 1.97 | 0.47 |
| 4:EH:202:LEU:HD21 | 4:EH:254:PHE:CZ | 2.50 | 0.47 |
| 4:EH:178:THR:HA | 4:EH:275:ALA:HA | 1.97 | 0.47 |
| 4:EG:54:THR:HA | 4:EH:7:LYS:O | 2.15 | 0.47 |
| 5:EJ:313:PHE:CE2 | 5:EJ:320:LEU:HD21 | 2.50 | 0.47 |
| 5:FA:110:VAL:HG22 | 5:FA:123:PRO:HB3 | 1.97 | 0.47 |
| 5:FA:139:ALA:HB3 | 5:FA:140:PRO:HD3 | 1.96 | 0.47 |
| 5:FA:339:GLU:HG3 | 5:FA:340:VAL:HG13 | 1.97 | 0.47 |
| 5:FA:356:TYR:HE1 | 6:FC:4:LEU:HD13 | 1.80 | 0.47 |
| 5:EJ:597:ARG:HH12 | 5:FA:489:GLY:N | 2.12 | 0.47 |
| 6:FB:168:LEU:HB2 | 6:FB:180:GLN:OE1 | 2.15 | 0.47 |
| 6:FD:168:LEU:HB2 | 6:FD:180:GLN:OE1 | 2.15 | 0.47 |
| 7:FE:100:TYR:CZ | 7:FF:113:GLU:HA | 2.49 | 0.47 |
| 7:FF:11:ASN:N | 7:FF:11:ASN:OD1 | 2.48 | 0.47 |
| 7:FF:445:HIS:CE1 | 7:FG:445:HIS:NE2 | 2.83 | 0.47 |
| 6:CI:184:SER:HA | 7:FG:149:GLN:OE1 | 2.15 | 0.47 |
| 7:FE:329:ASN:CG | 7:FG:333:THR:HB | 2.35 | 0.47 |
| 8:FH:112:ILE:HD11 | 8:FH:126:GLU:OE2 | 2.15 | 0.47 |
| 8:FI:112:ILE:HD11 | 8:FI:126:GLU:OE2 | 2.15 | 0.47 |
| 4:G:114:GLY:HA3 | 4:G:143:TYR:CE2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:178:THR:HA | 4:G:275:ALA:HA | 1.97 | 0.47 |
| 1:GE:143:TYR:CD2 | 1:GE:279:ASP:HB2 | 2.49 | 0.47 |
| 1:GE:209:TRP:HE3 | 1:GE:212:LYS:CB | 2.26 | 0.47 |
| 2:GF:16:LEU:HD23 | 2:GF:102:THR:HA | 1.97 | 0.47 |
| 2:GF:339:ASP:HB3 | 2:GF:340:PRO:CD | 2.36 | 0.47 |
| 2:GF:543:LYS:HE2 | 2:GF:574:LYS:O | 2.14 | 0.47 |
| 2:GF:808:GLN:HE21 | 2:GF:839:ILE:HG13 | 1.80 | 0.47 |
| 2:GF:912:ILE:HD11 | 3:GG:329:ASN:HD22 | 1.80 | 0.47 |
| 2:GF:91:GLN:HE21 | 2:GF:92:SER:H | 1.62 | 0.47 |
| 2:GF:928:GLU:HA | 2:GF:961:VAL:O | 2.14 | 0.47 |
| 3:GH:47:TRP:CD1 | 3:GH:270:ARG:HD2 | 2.50 | 0.47 |
| 4:GI:139:VAL:HG13 | 4:GI:164:ILE:HD12 | 1.97 | 0.47 |
| 4:GJ:200:ALA:HB3 | 4:GJ:221:ILE:HD11 | 1.96 | 0.47 |
| 4:HA:202:LEU:HD21 | 4:HA:254:PHE:CZ | 2.50 | 0.47 |
| 5:HB:117:ILE:HG22 | 5:HB:143:TRP:HE3 | 1.79 | 0.47 |
| 5:HB:206:PHE:CD2 | 5:HB:223:VAL:HA | 2.50 | 0.47 |
| 5:HB:255:ARG:CZ | 5:HD:390:LEU:HD12 | 2.44 | 0.47 |
| 5:HB:258:TYR:OH | 5:HB:260:ARG:HB2 | 2.14 | 0.47 |
| 5:HC:163:ALA:HB3 | 5:HC:246:THR:HG22 | 1.96 | 0.47 |
| 5:HC:258:TYR:O | 5:HC:259:THR:OG1 | 2.24 | 0.47 |
| 5:HC:288:MET:CE | 5:HC:292:PRO:HD3 | 2.44 | 0.47 |
| 5:HC:313:PHE:CE2 | 5:HC:320:LEU:HD21 | 2.50 | 0.47 |
| 5:HD:318:GLN:HB3 | 6:HF:4:LEU:CG | 2.45 | 0.47 |
| 6:HF:10:VAL:HA | 6:HG:13:ARG:HB2 | 1.95 | 0.47 |
| 7:HH:266:THR:HG23 | 7:HH:281:LEU:HD23 | 1.97 | 0.47 |
| 7:HJ:160:MET:HG2 | 7:HJ:165:THR:HB | 1.96 | 0.47 |
| 7:HJ:365:GLY:N | 7:HJ:392:LEU:HB2 | 2.29 | 0.47 |
| 5:I:359:GLU:O | 5:I:369:LEU:HA | 2.14 | 0.47 |
| 5:J:313:PHE:CE2 | 5:J:320:LEU:HD21 | 2.50 | 0.47 |
| 2:C:221:ALA:O | 5:J:564:PRO:HG2 | 2.14 | 0.47 |
| 5:J:526:THR:HG21 | 5:J:582:PRO:HB2 | 1.97 | 0.47 |
| 6:L:168:LEU:HB2 | 6:L:180:GLN:OE1 | 2.15 | 0.47 |
| 7:O:349:TRP:NE1 | 7:O:351:ALA:HB3 | 2.30 | 0.47 |
| 7:O:32:VAL:HA | 7:O:35:ALA:HB3 | 1.97 | 0.47 |
| 7:O:503:ASN:OD1 | 7:Q:446:LYS:N | 2.47 | 0.47 |
| 7:P:142:ILE:HG22 | 7:P:143:LYS:O | 2.14 | 0.47 |
| 7:P:359:TRP:CE2 | 7:P:524:LYS:HD3 | 2.50 | 0.47 |
| 7:Q:160:MET:HG2 | 7:Q:165:THR:HB | 1.96 | 0.47 |
| 8:R:79:HIS:CE1 | 8:R:151:GLN:HE22 | 2.33 | 0.47 |
| 11:V:190:LYS:O | 11:V:193:GLY:N | 2.48 | 0.47 |
| 12:W:120:SER:HA | 12:W:123:LEU:HG | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:200:TYR:HB2 | 1:X:269:VAL:CG1 | 2.44 | 0.47 |
| 1:X:67:ILE:CD1 | 1:Y:67:ILE:HG21 | 2.45 | 0.47 |
| 1:Y:144:ASN:OD1 | 1:Y:144:ASN:N | 2.47 | 0.47 |
| 13:YA:370[E]:ASN:ND2 | 13:YA:372[E]:SER:HB3 | 2.30 | 0.47 |
| 13:YA:464[A]:TYR:OH | 13:YC:454[A]:LYS:NZ | 2.48 | 0.47 |
| 13:YA:550[E]:TRP:O | 13:YC:558[E]:SER:N | 2.48 | 0.47 |
| 13:YA:81[B]:ARG:HB3 | 13:YA:100[B]:TYR:CZ | 2.50 | 0.47 |
| 13:YB:39[B]:ARG:NH1 | 13:YB:113[B]:GLY:HA2 | 2.30 | 0.47 |
| 13:YB:158[F]:PRO:HB2 | 13:YC:473[F]:GLN:OE1 | 2.14 | 0.47 |
| 13:YB:257[D]:LYS:HE2 | 13:YB:266[D]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YB:379[A]:PRO:HG2 | 13:YB:429[A]:ARG:NE | 2.30 | 0.47 |
| 13:YB:69[C]:ILE:HG12 | 13:YC:396[C]:GLU:HA | 1.96 | 0.47 |
| 13:YC:12[B]:VAL:HG21 | 14:YE:256[B]:HIS:CE1 | 2.50 | 0.47 |
| 13:YC:257[F]:LYS:HE2 | 13:YC:266[F]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YC:337[F]:GLU:O | 13:YC:340[F]:GLY:N | 2.48 | 0.47 |
| 13:YA:447[A]:ASN:HB3 | 13:YC:376[A]:PHE:CZ | 2.50 | 0.47 |
| 13:YA:464[E]:TYR:OH | 13:YC:454[E]:LYS:NZ | 2.47 | 0.47 |
| 13:YA:450[A]:VAL:O | 13:YC:459[A]:GLY:N | 2.48 | 0.47 |
| 13:YB:158[D]:PRO:HB2 | 13:YC:473[D]:GLN:OE1 | 2.14 | 0.47 |
| 13:YB:574[C]:ILE:HG22 | 13:YC:572[C]:ILE:HD13 | 1.97 | 0.47 |
| 14:YD:101[B]:GLY:HA3 | 14:YF:330[B]:LYS:HG2 | 1.97 | 0.47 |
| 14:YE:185[E]:PHE:CD2 | 14:YE:297[E]:ARG:HA | 2.49 | 0.47 |
| 14:YE:31[E]:LEU:O | 14:YE:35[E]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:185[C]:PHE:CD2 | 14:YF:297[C]:ARG:HA | 2.49 | 0.47 |
| 14:YF:214[A]:GLY:O | 14:YF:215[A]:GLU:HG3 | 2.15 | 0.47 |
| 15:ZA:66[E]:LYS:O | 15:ZA:68[E]:TYR:CD1 | 2.68 | 0.47 |
| 1:A:472:ASP:C | 1:A:474:SER:H | 2.18 | 0.47 |
| 4:AB:178:THR:HA | 4:AB:275:ALA:HA | 1.97 | 0.47 |
| 5:AC:196:ARG:HG2 | 5:AE:198:ASN:O | 2.15 | 0.47 |
| 5:AC:478:TRP:CH2 | 5:AC:600:ARG:HB2 | 2.50 | 0.47 |
| 5:AD:170:GLU:O | 5:AD:172:GLN:N | 2.48 | 0.47 |
| 5:AD:247:PHE:HZ | 5:AE:162:VAL:HG21 | 1.78 | 0.47 |
| 5:AC:317:LEU:HD21 | 5:AD:260:ARG:NH2 | 2.30 | 0.47 |
| 5:AE:339:GLU:HG3 | 5:AE:340:VAL:HG13 | 1.97 | 0.47 |
| 7:AI:12:GLU:HG3 | 7:AI:15:TYR:H | 1.80 | 0.47 |
| 1:B:37:LEU:HD11 | 1:B:53:LEU:HD21 | 1.97 | 0.47 |
| 7:BA:383:TYR:CE1 | 7:BA:393:PRO:HG3 | 2.50 | 0.47 |
| 8:BB:79:HIS:HE1 | 8:BB:151:GLN:HE22 | 1.63 | 0.47 |
| 8:BC:79:HIS:HE1 | 8:BC:151:GLN:HE22 | 1.63 | 0.47 |
| 10:BE:203:ARG:NH2 | 10:BE:356:ARG:HH12 | 2.13 | 0.47 |
| 12:BG:127:SER:HB3 | 12:BG:161:SER:HG | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:BG:187:GLY:O | 12:BG:188:LEU:HD12 | 2.14 | 0.47 |
| 2:BJ:231:TYR:CE1 | 2:BJ:391:ARG:HD3 | 2.48 | 0.47 |
| 2:BJ:881:ARG:NH2 | 2:BJ:882:PHE:HE1 | 2.13 | 0.47 |
| 2:BJ:928:GLU:HA | 2:BJ:961:VAL:O | 2.14 | 0.47 |
| 2:C:644:ASP:O | 11:V:84:TYR:OH | 2.33 | 0.47 |
| 2:C:777:LEU:HD12 | 2:C:778:THR:N | 2.30 | 0.47 |
| 3:CA:24:PHE:O | 3:CA:27:SER:OG | 2.19 | 0.47 |
| 3:CA:57:ALA:HB2 | 3:CB:7:ILE:HG12 | 1.97 | 0.47 |
| 3:CA:310:ILE:HB | 3:CB:16:PHE:HB2 | 1.96 | 0.47 |
| 4:CD:212:ARG:HG3 | 4:CD:213:LYS:HG3 | 1.96 | 0.47 |
| 4:CE:139:VAL:HG13 | 4:CE:164:ILE:HD12 | 1.97 | 0.47 |
| 2:BJ:1003:GLN:OE1 | 5:CF:10:VAL:HA | 2.15 | 0.47 |
| 5:CF:49:TRP:HZ3 | 5:CF:96:ARG:HD2 | 1.80 | 0.47 |
| 5:CG:189:ASN:HD21 | 5:CH:150:GLN:HE22 | 1.63 | 0.47 |
| 5:CG:460:TYR:CE2 | 5:CG:462:ASN:HB2 | 2.50 | 0.47 |
| 7:DB:12:GLU:HG3 | 7:DB:15:TYR:H | 1.79 | 0.47 |
| 7:DC:216:MET:SD | 7:DD:202:GLY:HA3 | 2.55 | 0.47 |
| 7:DC:347:MET:HE3 | 7:DC:347:MET:HB2 | 1.77 | 0.47 |
| 7:DC:411:ASN:O | 7:DC:415:ASN:ND2 | 2.48 | 0.47 |
| 7:DD:127:ASN:O | 7:DD:131:THR:HG23 | 2.15 | 0.47 |
| 7:DB:173:ILE:HD11 | 7:DD:174:ALA:HB2 | 1.97 | 0.47 |
| 8:DE:31:ASN:OD1 | 8:DE:32:PHE:N | 2.48 | 0.47 |
| 8:DE:55:ASN:HD22 | 8:IA:99:ILE:HD11 | 1.80 | 0.47 |
| 11:DI:111:TYR:HB3 | 11:DI:121:TYR:HD1 | 1.80 | 0.47 |
| 1:EA:145:PHE:HD2 | 1:EA:169:GLN:OE1 | 1.97 | 0.47 |
| 1:EA:472:ASP:C | 1:EA:474:SER:H | 2.18 | 0.47 |
| 1:EB:645:ASP:OD1 | 1:EB:645:ASP:N | 2.46 | 0.47 |
| 2:EC:177:GLN:HE22 | 2:EC:534:VAL:HG12 | 1.80 | 0.47 |
| 2:EC:406:LEU:CD1 | 2:EC:413:TRP:HA | 2.44 | 0.47 |
| 2:EC:853:ASP:OD1 | 2:EC:854:TYR:N | 2.47 | 0.47 |
| 2:EC:881:ARG:NH2 | 2:EC:882:PHE:HE1 | 2.13 | 0.47 |
| 3:ED:177:GLU:HG3 | 3:ED:179:THR:H | 1.80 | 0.47 |
| 4:EF:50:VAL:C | 4:EF:52:ASN:H | 2.17 | 0.47 |
| 4:EG:139:VAL:HG13 | 4:EG:164:ILE:HD12 | 1.97 | 0.47 |
| 5:EI:194:LYS:HB3 | 5:EI:196:ARG:H | 1.79 | 0.47 |
| 5:EI:258:TYR:OH | 5:EI:260:ARG:HB2 | 2.14 | 0.47 |
| 5:EI:317:LEU:HD21 | 5:EJ:260:ARG:NH2 | 2.29 | 0.47 |
| 5:EI:359:GLU:O | 5:EI:369:LEU:HA | 2.14 | 0.47 |
| 5:EJ:213:GLY:CA | 5:EJ:221:GLU:HB2 | 2.45 | 0.47 |
| 5:EJ:490:TRP:CD1 | 5:EJ:516:ALA:HA | 2.49 | 0.47 |
| 5:EI:569:TYR:HB2 | 5:EJ:550:VAL:HB | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:83:THR:HA | 4:H:63:ALA:HB3 | 1.95 | 0.47 |
| 5:FA:129:ARG:HG3 | 5:FA:130:PHE:H | 1.80 | 0.47 |
| 5:FA:362:GLU:HG2 | 5:FA:368:ILE:HG22 | 1.96 | 0.47 |
| 7:FE:172:LEU:O | 7:FE:175:GLN:HG2 | 2.15 | 0.47 |
| 7:FE:191:VAL:C | 7:FF:188:GLN:HA | 2.35 | 0.47 |
| 7:FE:476:ASP:OD2 | 7:FF:454:HIS:HE1 | 1.98 | 0.47 |
| 7:FE:302:ILE:HD12 | 7:FF:306:PHE:CZ | 2.50 | 0.47 |
| 7:FG:253:ARG:O | 7:FG:262:VAL:HG22 | 2.14 | 0.47 |
| 7:FE:308:ILE:HD11 | 7:FG:306:PHE:HB3 | 1.96 | 0.47 |
| 7:FG:31:ASP:CG | 7:FG:34:ALA:H | 2.18 | 0.47 |
| 7:FE:468:PHE:HB2 | 7:FG:479:ASN:O | 2.14 | 0.47 |
| 8:DE:21:PHE:CG | 8:FH:142:LEU:HD21 | 2.50 | 0.47 |
| 11:GB:38:ARG:HH11 | 11:GB:187:ILE:HD12 | 1.79 | 0.47 |
| 12:GC:31:SER:O | 12:GC:32:THR:OG1 | 2.30 | 0.47 |
| 1:GD:179:TYR:HD1 | 1:GD:185:ILE:HD11 | 1.80 | 0.47 |
| 1:GD:472:ASP:C | 1:GD:474:SER:H | 2.18 | 0.47 |
| 1:GD:525:ASN:HB3 | 1:GD:528:THR:HG21 | 1.96 | 0.47 |
| 1:GE:106:ALA:HB2 | 1:GE:280:ALA:CB | 2.45 | 0.47 |
| 1:GE:455:PHE:CD2 | 1:GE:456:ASN:N | 2.83 | 0.47 |
| 1:GE:227:ARG:NE | 2:GF:694:TYR:CZ | 2.80 | 0.47 |
| 3:GG:104:TYR:HE2 | 3:GG:165:ARG:HH21 | 1.63 | 0.47 |
| 4:GJ:178:THR:HA | 4:GJ:275:ALA:HA | 1.97 | 0.47 |
| 4:F:164:ILE:HG23 | 4:H:172:GLU:OE1 | 2.15 | 0.47 |
| 5:HB:160:SER:HB3 | 5:HC:161:ASN:ND2 | 2.20 | 0.47 |
| 5:HB:182:ARG:NH1 | 5:HC:299:ILE:HG12 | 2.30 | 0.47 |
| 5:HB:23:GLY:O | 5:HB:24:ILE:HB | 2.15 | 0.47 |
| 5:HC:213:GLY:CA | 5:HC:221:GLU:HB2 | 2.45 | 0.47 |
| 5:HC:48:ALA:O | 5:HC:49:TRP:HD1 | 1.97 | 0.47 |
| 5:HB:164:ARG:NH1 | 5:HD:192:ARG:HD3 | 2.30 | 0.47 |
| 5:HD:186:TYR:HD2 | 5:HD:227:GLY:HA2 | 1.80 | 0.47 |
| 5:HD:272:SER:OG | 6:HG:106:THR:N | 2.34 | 0.47 |
| 5:HD:326:MET:HE3 | 5:HD:326:MET:HB2 | 1.80 | 0.47 |
| 7:P:205:ARG:NH1 | 6:HE:218:THR:HB | 2.28 | 0.47 |
| 7:HH:12:GLU:HG3 | 7:HH:15:TYR:H | 1.80 | 0.47 |
| 7:HH:172:LEU:O | 7:HH:175:GLN:HG2 | 2.15 | 0.47 |
| 7:HH:329:ASN:HD21 | 7:HJ:335:ASN:H | 1.63 | 0.47 |
| 6:FB:184:SER:HA | 7:HJ:149:GLN:OE1 | 2.14 | 0.47 |
| 7:HJ:220:SER:HB2 | 7:HJ:228:ILE:HG12 | 1.97 | 0.47 |
| 7:HJ:329:ASN:OD1 | 7:HJ:330:ARG:N | 2.48 | 0.47 |
| 7:HI:399:PHE:CD1 | 7:HJ:401:ARG:HB3 | 2.50 | 0.47 |
| 7:HJ:61:PRO:HD3 | 7:HJ:74:LYS:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:196:ARG:HG2 | 5:K:198:ASN:O | 2.15 | 0.47 |
| 5:I:217:GLU:HB2 | 5:I:222:LEU:HB2 | 1.97 | 0.47 |
| 5:I:496:ASP:OD2 | 5:I:499:PHE:HB2 | 2.15 | 0.47 |
| 5:K:186:TYR:HE1 | 5:K:246:THR:HA | 1.78 | 0.47 |
| 5:K:340:VAL:HG22 | 6:L:173:THR:HA | 1.97 | 0.47 |
| 7:O:172:LEU:O | 7:O:175:GLN:HG2 | 2.15 | 0.47 |
| 7:O:255:SER:O | 7:O:278:SER:OG | 2.29 | 0.47 |
| 7:P:347:MET:CE | 7:Q:345:ALA:HB1 | 2.45 | 0.47 |
| 7:P:516:ASN:ND2 | 7:Q:401:ARG:HD2 | 2.30 | 0.47 |
| 7:Q:329:ASN:OD1 | 7:Q:330:ARG:N | 2.48 | 0.47 |
| 7:Q:383:TYR:CE1 | 7:Q:393:PRO:HG3 | 2.50 | 0.47 |
| 11:V:135:ASP:CG | 11:V:136:LYS:N | 2.67 | 0.47 |
| 11:V:14:LYS:HE2 | 11:V:19:ASN:HA | 1.95 | 0.47 |
| 1:X:102:SER:OG | 1:X:103:LYS:N | 2.48 | 0.47 |
| 1:X:110:ILE:CD1 | 1:X:302:GLU:HA | 2.44 | 0.47 |
| 1:X:116:ASP:OD1 | 1:X:118:LEU:N | 2.46 | 0.47 |
| 1:X:210:THR:HG22 | 1:X:226:MET:H | 1.79 | 0.47 |
| 1:X:243:ILE:HG22 | 1:X:258:GLY:CA | 2.45 | 0.47 |
| 1:X:518:ASN:HA | 1:X:535:LEU:HB3 | 1.96 | 0.47 |
| 1:Y:106:ALA:HB2 | 1:Y:280:ALA:CB | 2.45 | 0.47 |
| 1:Y:645:ASP:OD1 | 1:Y:645:ASP:N | 2.46 | 0.47 |
| 13:YA:179[F]:MET:SD | 13:YA:279[F]:ASN:ND2 | 2.75 | 0.47 |
| 13:YA:257[D]:LYS:HE2 | 13:YA:266[D]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YA:337[D]:GLU:O | 13:YA:340[D]:GLY:N | 2.48 | 0.47 |
| 13:YA:461[D]:SER:HA | 13:YC:468[D]:ASP:HB3 | 1.96 | 0.47 |
| 13:YA:70[D]:GLY:O | 13:YB:393[D]:MET:HA | 2.14 | 0.47 |
| 13:YB:121[B]:TYR:OH | 13:YB:123[B]:ARG:NH2 | 2.48 | 0.47 |
| 13:YB:307[A]:ALA:HB1 | 13:YB:331[A]:ILE:HD11 | 1.95 | 0.47 |
| 13:YA:315[E]:LEU:HD23 | 13:YB:367[E]:PRO:HA | 1.95 | 0.47 |
| 13:YB:492[F]:GLY:HA3 | 13:YC:485[F]:ASP:HA | 1.97 | 0.47 |
| 13:YA:571[E]:ARG:HD3 | 13:YB:564[E]:GLN:HE22 | 1.80 | 0.47 |
| 13:YC:179[B]:MET:SD | 13:YC:279[B]:ASN:ND2 | 2.76 | 0.47 |
| 13:YA:452[C]:GLY:CA | 13:YC:321[C]:LYS:HD3 | 2.40 | 0.47 |
| 13:YA:447[B]:ASN:HB3 | 13:YC:376[B]:PHE:CZ | 2.50 | 0.47 |
| 13:YB:481[D]:PHE:O | 13:YC:473[D]:GLN:HA | 2.15 | 0.47 |
| 14:YD:189[C]:TRP:CD1 | 14:YD:320[C]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:244[A]:LYS:O | 14:YD:247[A]:PRO:HD2 | 2.14 | 0.47 |
| 13:YB:44[E]:VAL:HG11 | 14:YD:272[E]:GLU:HB3 | 1.95 | 0.47 |
| 14:YD:336[F]:GLU:O | 14:YD:359[F]:THR:OG1 | 2.33 | 0.47 |
| 14:YD:38[A]:LEU:HD12 | 14:YD:38[A]:LEU:HA | 1.63 | 0.47 |
| 1:GD:130:ARG:HD3 | 14:YE:181[D]:GLY:HA2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:189[E]:TRP:CD1 | 14:YE:320[E]:PRO:HG2 | 2.50 | 0.47 |
| 14:YE:244[C]:LYS:O | 14:YE:247[C]:PRO:HD2 | 2.14 | 0.47 |
| 13:YC:12[C]:VAL:HG21 | 14:YE:256[C]:HIS:CE1 | 2.50 | 0.47 |
| 11:IE:182:ASN:ND2 | 14:YE:327[D]:ASN:HD22 | 2.13 | 0.47 |
| 14:YE:336[D]:GLU:O | 14:YE:359[D]:THR:OG1 | 2.33 | 0.47 |
| 14:YE:54[C]:PHE:CZ | 14:YE:105[C]:ILE:HD11 | 2.48 | 0.47 |
| 1:GD:130:ARG:HD3 | 14:YF:181[B]:GLY:HA2 | 1.94 | 0.47 |
| 14:YF:189[B]:TRP:CD1 | 14:YF:320[B]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:95[C]:VAL:O | 14:YF:236[C]:TRP:N | 2.47 | 0.47 |
| 14:YF:31[F]:LEU:O | 14:YF:35[F]:ILE:HG22 | 2.14 | 0.47 |
| 14:YF:38[C]:LEU:HD12 | 14:YF:38[C]:LEU:HA | 1.63 | 0.47 |
| 14:YF:72[D]:ILE:O | 14:YF:86[D]:ARG:N | 2.47 | 0.47 |
| 14:YF:72[C]:ILE:O | 14:YF:86[C]:ARG:N | 2.47 | 0.47 |
| 2:Z:406:LEU:CD1 | 2:Z:413:TRP:HA | 2.44 | 0.47 |
| 1:A:508:ARG:HH22 | 1:A:577:PHE:CA | 2.27 | 0.47 |
| 1:A:518:ASN:HA | 1:A:535:LEU:HB3 | 1.96 | 0.47 |
| 4:AA:178:THR:HA | 4:AA:275:ALA:HA | 1.97 | 0.47 |
| 5:AC:359:GLU:O | 5:AC:369:LEU:HA | 2.14 | 0.47 |
| 5:AD:258:TYR:O | 5:AD:259:THR:OG1 | 2.24 | 0.47 |
| 5:AD:313:PHE:CE2 | 5:AD:320:LEU:HD21 | 2.50 | 0.47 |
| 5:AE:186:TYR:HD2 | 5:AE:227:GLY:HA2 | 1.80 | 0.47 |
| 5:AC:239:GLY:O | 7:AI:2:SER:N | 2.48 | 0.47 |
| 7:AI:321:MET:HA | 7:BA:315:ILE:O | 2.15 | 0.47 |
| 7:AJ:141:VAL:HG22 | 7:BA:139:ASN:HB2 | 1.96 | 0.47 |
| 1:B:175:THR:O | 1:B:270:ILE:HG22 | 2.15 | 0.47 |
| 1:B:106:ALA:HB2 | 1:B:280:ALA:CB | 2.45 | 0.47 |
| 8:BB:79:HIS:CE1 | 8:BB:151:GLN:HE22 | 2.33 | 0.47 |
| 10:BE:323:LYS:O | 10:BE:324:THR:OG1 | 2.33 | 0.47 |
| 11:BF:74:LEU:HD11 | 11:BF:79:ASN:HD21 | 1.79 | 0.47 |
| 1:BI:118:LEU:HG | 1:BI:294:ASN:CG | 2.35 | 0.47 |
| 2:BJ:254:PHE:HB3 | 2:BJ:294:PHE:HB3 | 1.97 | 0.47 |
| 2:BJ:777:LEU:HD12 | 2:BJ:778:THR:N | 2.30 | 0.47 |
| 2:BJ:923:SER:HB3 | 2:BJ:992:PRO:HG2 | 1.96 | 0.47 |
| 2:C:151:PHE:CD2 | 2:C:166:PHE:HE1 | 2.33 | 0.47 |
| 2:C:706:SER:O | 2:C:708:ILE:N | 2.42 | 0.47 |
| 3:CA:42:GLY:HA2 | 3:CA:76:MET:HG3 | 1.97 | 0.47 |
| 3:CB:71:MET:HG3 | 3:CB:271:GLN:NE2 | 2.29 | 0.47 |
| 4:CC:139:VAL:HG13 | 4:CC:164:ILE:HD12 | 1.97 | 0.47 |
| 4:CC:205:THR:HG22 | 4:CD:284:ILE:HD11 | 1.96 | 0.47 |
| 4:CC:164:ILE:HG23 | 4:CE:172:GLU:OE1 | 2.15 | 0.47 |
| 5:CF:170:GLU:O | 5:CF:172:GLN:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:359:GLU:O | 5:CF:369:LEU:HA | 2.14 | 0.47 |
| 5:CF:97:ASP:HB3 | 5:CF:99:PHE:O | 2.13 | 0.47 |
| 5:CG:321:ALA:HA | 5:CG:358:VAL:HB | 1.95 | 0.47 |
| 5:CG:326:MET:HB2 | 5:CG:326:MET:HE3 | 1.70 | 0.47 |
| 6:DA:127:ALA:HA | 6:DA:130:ARG:HH11 | 1.79 | 0.47 |
| 7:DC:119:ALA:O | 7:DC:122:THR:OG1 | 2.24 | 0.47 |
| 7:DD:375:TYR:CZ | 7:DD:392:LEU:HD23 | 2.50 | 0.47 |
| 7:DB:39:ILE:HA | 7:DD:44:VAL:HG22 | 1.95 | 0.47 |
| 8:BB:115:GLN:HG2 | 8:DE:79:HIS:HE2 | 1.79 | 0.47 |
| 8:DF:31:ASN:OD1 | 8:DF:32:PHE:N | 2.48 | 0.47 |
| 10:DH:334:ILE:HG13 | 10:DH:335:ALA:N | 2.30 | 0.47 |
| 10:DH:330:ASN:HB2 | 12:DJ:189:ARG:NH2 | 2.30 | 0.47 |
| 12:DJ:214:VAL:HG23 | 12:DJ:249:GLN:O | 2.15 | 0.47 |
| 1:EA:518:ASN:HA | 1:EA:535:LEU:HB3 | 1.96 | 0.47 |
| 1:EB:372:ALA:N | 1:EB:404:ILE:HD11 | 2.30 | 0.47 |
| 1:EB:455:PHE:CD2 | 1:EB:456:ASN:N | 2.83 | 0.47 |
| 1:EB:363:PHE:CG | 1:EB:636:ASP:HB2 | 2.50 | 0.47 |
| 1:EB:76:TYR:CE1 | 11:GB:31:ASN:HB3 | 2.50 | 0.47 |
| 2:EC:340:PRO:HA | 2:EC:345:TYR:CD1 | 2.50 | 0.47 |
| 2:EC:525:TRP:CE2 | 2:EC:526:ILE:O | 2.68 | 0.47 |
| 2:EC:777:LEU:HD12 | 2:EC:778:THR:N | 2.30 | 0.47 |
| 3:ED:131:TYR:CE1 | 3:ED:190:TYR:HD1 | 2.33 | 0.47 |
| 3:ED:57:ALA:HB2 | 3:EE:7:ILE:HG12 | 1.97 | 0.47 |
| 4:EF:7:LYS:HE2 | 4:EH:53:GLY:HA3 | 1.97 | 0.47 |
| 5:EI:313:PHE:HE2 | 5:EI:320:LEU:HD11 | 1.80 | 0.47 |
| 5:EI:478:TRP:CH2 | 5:EI:600:ARG:HB2 | 2.50 | 0.47 |
| 5:EJ:163:ALA:HB3 | 5:EJ:246:THR:HG22 | 1.96 | 0.47 |
| 5:EJ:204:ASP:OD1 | 5:EJ:205:VAL:N | 2.41 | 0.47 |
| 4:F:50:VAL:C | 4:F:52:ASN:H | 2.17 | 0.47 |
| 5:FA:86:VAL:HG13 | 5:FA:87:ASN:N | 2.29 | 0.47 |
| 6:FD:125:PHE:O | 6:FD:129:VAL:HG23 | 2.14 | 0.47 |
| 7:FE:195:THR:O | 7:FE:198:GLN:N | 2.48 | 0.47 |
| 7:FE:84:ARG:NH1 | 7:FG:85:LEU:HD22 | 2.29 | 0.47 |
| 8:FH:79:HIS:CE1 | 8:FH:151:GLN:HE22 | 2.33 | 0.47 |
| 8:FI:85:PHE:HB3 | 8:FI:137:VAL:HG21 | 1.96 | 0.47 |
| 12:GC:21:MET:HB3 | 12:GC:204:HIS:O | 2.15 | 0.47 |
| 1:GD:52:ARG:NH2 | 9:IC:25:ARG:HB3 | 2.30 | 0.47 |
| 1:GD:543:THR:HG23 | 1:GD:544:ASP:O | 2.15 | 0.47 |
| 1:GE:619:GLN:N | 1:GE:619:GLN:OE1 | 2.35 | 0.47 |
| 1:GE:645:ASP:OD1 | 1:GE:645:ASP:N | 2.46 | 0.47 |
| 2:GF:228:ARG:HB3 | 2:GF:250:TYR:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:664:PHE:O | 2:GF:667:PHE:HB3 | 2.15 | 0.47 |
| 2:GF:881:ARG:NH2 | 2:GF:882:PHE:HE1 | 2.13 | 0.47 |
| 3:GG:131:TYR:CE1 | 3:GG:190:TYR:HD1 | 2.33 | 0.47 |
| 3:GG:174:GLY:HA3 | 3:GG:180:ILE:HG12 | 1.97 | 0.47 |
| 2:GF:986:ARG:HH22 | 3:GG:323:ASP:HB2 | 1.79 | 0.47 |
| 4:HA:139:VAL:HG13 | 4:HA:164:ILE:HD12 | 1.97 | 0.47 |
| 4:HA:212:ARG:HG3 | 4:HA:213:LYS:HG3 | 1.96 | 0.47 |
| 5:HB:339:GLU:HG3 | 5:HB:340:VAL:HG13 | 1.96 | 0.47 |
| 5:HC:261:ARG:N | 5:HC:383:ILE:O | 2.35 | 0.47 |
| 5:HC:506:LEU:HD23 | 5:HC:512:PRO:HA | 1.96 | 0.47 |
| 5:HB:591:PRO:HA | 5:HC:520:GLY:O | 2.14 | 0.47 |
| 5:HD:117:ILE:HG22 | 5:HD:143:TRP:HE3 | 1.80 | 0.47 |
| 5:HD:190:ASN:HB2 | 5:HD:247:PHE:HB2 | 1.95 | 0.47 |
| 5:HD:207:SER:O | 5:HD:210:SER:OG | 2.32 | 0.47 |
| 6:HF:168:LEU:HB2 | 6:HF:180:GLN:OE1 | 2.15 | 0.47 |
| 7:HI:368:SER:HA | 7:HI:389:ASN:HD22 | 1.79 | 0.47 |
| 7:HI:359:TRP:CE2 | 7:HI:524:LYS:HD3 | 2.50 | 0.47 |
| 5:I:486:VAL:HG12 | 5:J:488:VAL:HG22 | 1.96 | 0.47 |
| 8:IA:79:HIS:CE1 | 8:IA:151:GLN:HE22 | 2.33 | 0.47 |
| 8:IA:130:LYS:NZ | 8:IA:163:GLU:OE2 | 2.37 | 0.47 |
| 8:IB:79:HIS:HE1 | 8:IB:151:GLN:HE22 | 1.63 | 0.47 |
| 11:IE:135:ASP:CG | 11:IE:136:LYS:N | 2.67 | 0.47 |
| 5:J:170:GLU:O | 5:J:171:VAL:HG12 | 2.14 | 0.47 |
| 5:J:169:VAL:O | 5:J:238:ILE:HA | 2.15 | 0.47 |
| 5:J:358:VAL:HA | 5:J:371:PHE:HA | 1.96 | 0.47 |
| 7:O:342:PRO:HG2 | 7:O:345:ALA:HB2 | 1.96 | 0.47 |
| 7:O:418:ASP:OD2 | 7:P:505:PRO:HD3 | 2.14 | 0.47 |
| 7:O:401:ARG:NH2 | 7:Q:397:GLY:O | 2.48 | 0.47 |
| 7:P:399:PHE:CD1 | 7:Q:401:ARG:HB3 | 2.50 | 0.47 |
| 1:Y:538:VAL:HG11 | 1:Y:558:PHE:HE1 | 1.80 | 0.47 |
| 1:Y:572:TYR:HB2 | 1:Y:591:VAL:HG23 | 1.97 | 0.47 |
| 13:YA:189[A]:LYS:HA | 13:YA:234[A]:GLY:O | 2.14 | 0.47 |
| 13:YA:257[A]:LYS:HE2 | 13:YA:266[A]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YA:257[E]:LYS:HE2 | 13:YA:266[E]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YA:394[B]:GLU:N | 13:YC:70[B]:GLY:O | 2.47 | 0.47 |
| 13:YA:39[D]:ARG:NH1 | 13:YA:113[D]:GLY:HA2 | 2.30 | 0.47 |
| 13:YA:379[C]:PRO:HG2 | 13:YA:429[C]:ARG:NE | 2.29 | 0.47 |
| 13:YB:189[A]:LYS:HA | 13:YB:234[A]:GLY:O | 2.14 | 0.47 |
| 13:YB:492[C]:GLY:HA3 | 13:YC:485[C]:ASP:HA | 1.97 | 0.47 |
| 13:YC:189[E]:LYS:HA | 13:YC:234[E]:GLY:O | 2.14 | 0.47 |
| 13:YC:252[D]:MET:HE3 | 13:YC:252[D]:MET:HB3 | 1.81 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:257[B]:LYS:HE2 | 13:YC:266[B]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YC:307[A]:ALA:HB1 | 13:YC:331[A]:ILE:HD11 | 1.95 | 0.47 |
| 13:YC:337[E]:GLU:O | 13:YC:340[E]:GLY:N | 2.48 | 0.47 |
| 13:YC:370[F]:ASN:ND2 | 13:YC:372[F]:SER:HB3 | 2.29 | 0.47 |
| 13:YC:39[A]:ARG:NH1 | 13:YC:113[A]:GLY:HA2 | 2.30 | 0.47 |
| 13:YA:461[E]:SER:HA | 13:YC:468[E]:ASP:HB3 | 1.96 | 0.47 |
| 13:YB:158[E]:PRO:HB2 | 13:YC:473[E]:GLN:OE1 | 2.14 | 0.47 |
| 13:YA:470[F]:ARG:HD2 | 13:YC:474[F]:ILE:HD11 | 1.96 | 0.47 |
| 13:YB:546[F]:VAL:HA | 13:YC:538[F]:VAL:O | 2.14 | 0.47 |
| 13:YA:122[F]:PRO:HB3 | 13:YC:66[F]:MET:HE2 | 1.96 | 0.47 |
| 14:YD:140[C]:TYR:CD2 | 14:YD:147[C]:THR:HA | 2.50 | 0.47 |
| 14:YD:185[F]:PHE:CD2 | 14:YD:297[F]:ARG:HA | 2.49 | 0.47 |
| 14:YD:332[F]:GLN:HB3 | 14:YE:61[F]:HIS:NE2 | 2.30 | 0.47 |
| 14:YE:109[A]:LEU:HA | 14:YE:109[A]:LEU:HD12 | 1.65 | 0.47 |
| 14:YE:140[A]:TYR:CD2 | 14:YE:147[A]:THR:HA | 2.50 | 0.47 |
| 14:YE:14[F]:VAL:HG11 | 14:YE:52[F]:LEU:HD11 | 1.96 | 0.47 |
| 14:YE:189[A]:TRP:CD1 | 14:YE:320[A]:PRO:HG2 | 2.50 | 0.47 |
| 14:YE:212[E]:ILE:HG22 | 14:YE:327[E]:ASN:HB2 | 1.97 | 0.47 |
| 14:YE:214[A]:GLY:O | 14:YE:215[A]:GLU:HG3 | 2.15 | 0.47 |
| 14:YE:244[E]:LYS:O | 14:YE:247[E]:PRO:HD2 | 2.14 | 0.47 |
| 14:YE:189[B]:TRP:CD1 | 14:YE:320[B]:PRO:HG2 | 2.50 | 0.47 |
| 14:YD:236[D]:TRP:N | 14:YE:95[D]:VAL:O | 2.48 | 0.47 |
| 14:YF:10[E]:PRO:HD2 | 14:YF:349[E]:ASN:O | 2.15 | 0.47 |
| 14:YF:14[D]:VAL:HG11 | 14:YF:52[D]:LEU:HD11 | 1.96 | 0.47 |
| 14:YF:214[E]:GLY:O | 14:YF:215[E]:GLU:HG3 | 2.15 | 0.47 |
| 14:YF:244[A]:LYS:O | 14:YF:247[A]:PRO:HD2 | 2.14 | 0.47 |
| 14:YF:31[C]:LEU:O | 14:YF:35[C]:ILE:HG22 | 2.14 | 0.47 |
| 2:Z:149:GLU:O | 2:Z:150:SER:OG | 2.18 | 0.47 |
| 2:Z:555:ARG:HG3 | 2:Z:557:VAL:N | 2.29 | 0.47 |
| 2:Z:928:GLU:HA | 2:Z:961:VAL:O | 2.14 | 0.47 |
| 15:ZA:66[C]:LYS:O | 15:ZA:68[C]:TYR:CD1 | 2.68 | 0.47 |
| 1:A:179:TYR:HD1 | 1:A:185:ILE:HD11 | 1.80 | 0.47 |
| 1:A:252:LEU:HD12 | 1:A:252:LEU:O | 2.15 | 0.47 |
| 1:A:243:ILE:HG22 | 1:A:258:GLY:CA | 2.45 | 0.47 |
| 1:A:345:TYR:OH | 1:A:400:ASN:CG | 2.54 | 0.47 |
| 1:A:436:LEU:O | 1:A:439:GLN:N | 2.47 | 0.47 |
| 5:AC:217:GLU:HB2 | 5:AC:222:LEU:HB2 | 1.97 | 0.47 |
| 5:AD:460:TYR:CE2 | 5:AD:462:ASN:HB2 | 2.50 | 0.47 |
| 5:AD:48:ALA:O | 5:AD:49:TRP:HD1 | 1.97 | 0.47 |
| 5:AE:63:GLU:HB2 | 5:AE:68:TYR:OH | 2.14 | 0.47 |
| 1:B:23:GLY:O | 1:B:29:ILE:HD11 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BA:335:ASN:OD1 | 7:BA:336:GLU:N | 2.47 | 0.47 |
| 7:BA:61:PRO:HD3 | 7:BA:74:LYS:HB3 | 1.97 | 0.47 |
| 11:BF:190:LYS:O | 11:BF:193:GLY:N | 2.48 | 0.47 |
| 12:BG:153:ARG:HH22 | 12:DJ:184:PRO:HA | 1.80 | 0.47 |
| 1:BH:345:TYR:OH | 1:BH:400:ASN:CG | 2.54 | 0.47 |
| 1:BI:194:ARG:HA | 1:BI:197:VAL:HG23 | 1.97 | 0.47 |
| 1:BI:200:TYR:HB2 | 1:BI:269:VAL:HG13 | 1.97 | 0.47 |
| 2:BJ:182:GLN:N | 2:BJ:182:GLN:OE1 | 2.41 | 0.47 |
| 2:BJ:507:LYS:O | 3:EE:176:ALA:HB2 | 2.15 | 0.47 |
| 2:BJ:548:ILE:N | 2:BJ:549:PRO:HD3 | 2.30 | 0.47 |
| 2:C:406:LEU:CD1 | 2:C:413:TRP:HA | 2.44 | 0.47 |
| 2:C:654:PRO:HG3 | 9:T:47:ARG:CD | 2.45 | 0.47 |
| 2:C:881:ARG:NH2 | 2:C:882:PHE:HE1 | 2.13 | 0.47 |
| 4:CD:178:THR:HA | 4:CD:275:ALA:HA | 1.97 | 0.47 |
| 5:CF:186:TYR:HB3 | 5:CF:227:GLY:O | 2.14 | 0.47 |
| 5:CF:326:MET:HE3 | 5:CF:326:MET:HB2 | 1.81 | 0.47 |
| 5:CG:19:LEU:HD13 | 5:CH:19:LEU:HD21 | 1.97 | 0.47 |
| 5:CH:339:GLU:HG3 | 5:CH:340:VAL:HG13 | 1.97 | 0.47 |
| 6:CI:76:GLY:HA2 | 6:CI:215:PHE:HZ | 1.80 | 0.47 |
| 3:D:104:TYR:HE2 | 3:D:165:ARG:HH21 | 1.63 | 0.47 |
| 3:D:177:GLU:HG3 | 3:D:179:THR:H | 1.80 | 0.47 |
| 7:DB:110:VAL:HG12 | 7:DB:111:ASN:N | 2.30 | 0.47 |
| 7:DB:263:VAL:O | 7:DC:260:ARG:HA | 2.15 | 0.47 |
| 7:DD:220:SER:OG | 7:DD:226:GLY:O | 2.33 | 0.47 |
| 7:DC:335:ASN:H | 7:DD:329:ASN:HD21 | 1.63 | 0.47 |
| 8:BB:117:ALA:HA | 8:DE:77:GLU:OE2 | 2.15 | 0.47 |
| 8:DF:121:LYS:HZ2 | 8:DF:122:THR:HG1 | 1.63 | 0.47 |
| 12:DJ:223:VAL:HB | 12:DJ:241:VAL:HG23 | 1.97 | 0.47 |
| 3:E:64:SER:HG | 3:E:67:GLY:H | 1.57 | 0.47 |
| 1:EA:200:TYR:HB2 | 1:EA:269:VAL:CG1 | 2.44 | 0.47 |
| 1:EA:227:ARG:HB2 | 1:EA:237:TYR:CE2 | 2.50 | 0.47 |
| 1:EA:543:THR:HG23 | 1:EA:544:ASP:O | 2.15 | 0.47 |
| 2:EC:213:ASN:HB2 | 2:EC:289:PHE:CE1 | 2.49 | 0.47 |
| 2:EC:340:PRO:O | 2:EC:342:SER:N | 2.46 | 0.47 |
| 2:EC:528:ASN:HB3 | 3:GH:233:GLN:NE2 | 2.30 | 0.47 |
| 1:EB:227:ARG:NE | 2:EC:694:TYR:CZ | 2.80 | 0.47 |
| 2:EC:938:PRO:HD2 | 2:EC:943:GLU:HB2 | 1.97 | 0.47 |
| 3:EE:321:ALA:O | 3:EE:324:GLN:HB3 | 2.15 | 0.47 |
| 4:EF:202:LEU:HD21 | 4:EF:254:PHE:CZ | 2.50 | 0.47 |
| 5:EJ:358:VAL:HA | 5:EJ:371:PHE:HA | 1.97 | 0.47 |
| 5:EJ:460:TYR:CE2 | 5:EJ:462:ASN:HB2 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:526:THR:HG21 | 5:EJ:582:PRO:HB2 | 1.97 | 0.47 |
| 5:FA:104:VAL:HG13 | 5:FA:105:ASN:H | 1.80 | 0.47 |
| 5:FA:344:VAL:HG12 | 5:FA:349:TRP:H | 1.80 | 0.47 |
| 7:FF:117:THR:OG1 | 7:FG:112:ASN:HA | 2.15 | 0.47 |
| 7:FG:325:TYR:CD1 | 7:FG:330:ARG:HA | 2.45 | 0.47 |
| 7:FG:365:GLY:CA | 7:FG:392:LEU:HB2 | 2.45 | 0.47 |
| 8:FI:79:HIS:CE1 | 8:FI:151:GLN:HE22 | 2.33 | 0.47 |
| 4:G:39:TYR:CG | 4:H:7:LYS:HD3 | 2.49 | 0.47 |
| 1:GD:102:SER:OG | 1:GD:103:LYS:N | 2.48 | 0.47 |
| 1:GD:436:LEU:O | 1:GD:439:GLN:N | 2.47 | 0.47 |
| 1:GD:444:ILE:O | 1:GD:447:TYR:HB3 | 2.15 | 0.47 |
| 2:GF:180:ILE:HG23 | 2:GF:201:LEU:HD11 | 1.97 | 0.47 |
| 2:GF:357:ILE:HG23 | 2:GF:358:THR:N | 2.30 | 0.47 |
| 3:D:47:TRP:HB2 | 2:GF:454:ASN:ND2 | 2.30 | 0.47 |
| 2:GF:494:GLU:HB2 | 2:GF:498:TRP:HB2 | 1.96 | 0.47 |
| 2:GF:525:TRP:CE2 | 2:GF:526:ILE:O | 2.68 | 0.47 |
| 2:GF:712:ASN:HA | 2:GF:751:LEU:HG | 1.97 | 0.47 |
| 3:GG:232:GLN:N | 3:GG:232:GLN:OE1 | 2.42 | 0.47 |
| 3:GG:257:TYR:HB3 | 3:GG:296:TYR:CE2 | 2.50 | 0.47 |
| 3:GG:47:TRP:HZ3 | 3:GG:270:ARG:HD3 | 1.79 | 0.47 |
| 2:EC:454:ASN:ND2 | 3:GG:47:TRP:HB2 | 2.30 | 0.47 |
| 3:GH:321:ALA:O | 3:GH:324:GLN:HB3 | 2.15 | 0.47 |
| 4:GJ:139:VAL:HG13 | 4:GJ:164:ILE:HD12 | 1.97 | 0.47 |
| 4:GJ:39:TYR:CG | 4:HA:7:LYS:HD3 | 2.50 | 0.47 |
| 4:H:67:TYR:CD1 | 4:H:84:ARG:HB3 | 2.50 | 0.47 |
| 4:HA:114:GLY:HA3 | 4:HA:143:TYR:CE2 | 2.49 | 0.47 |
| 5:HB:196:ARG:O | 5:HD:197:GLY:HA2 | 2.14 | 0.47 |
| 5:HB:391:GLY:O | 5:HB:392:THR:OG1 | 2.23 | 0.47 |
| 5:HC:147:LYS:HG2 | 5:HD:154:ILE:O | 2.14 | 0.47 |
| 5:HC:169:VAL:O | 5:HC:238:ILE:HA | 2.15 | 0.47 |
| 5:HC:250:GLY:N | 5:HD:158:ASP:HB3 | 2.30 | 0.47 |
| 5:HB:182:ARG:HH22 | 5:HC:299:ILE:HG21 | 1.80 | 0.47 |
| 5:HC:290:SER:CB | 5:HC:371:PHE:H | 2.27 | 0.47 |
| 5:HB:486:VAL:HG12 | 5:HC:488:VAL:HG22 | 1.96 | 0.47 |
| 5:HD:196:ARG:HD2 | 7:HI:5:THR:OG1 | 2.15 | 0.47 |
| 6:HF:69:THR:HA | 6:HG:73:ASN:CB | 2.45 | 0.47 |
| 6:HE:10:VAL:CG1 | 6:HG:10:VAL:HG21 | 2.45 | 0.47 |
| 7:HH:60:ILE:HG22 | 7:HI:52:SER:N | 2.30 | 0.47 |
| 7:HI:11:ASN:OD1 | 7:HI:11:ASN:N | 2.48 | 0.47 |
| 7:HI:347:MET:CE | 7:HJ:345:ALA:HB1 | 2.45 | 0.47 |
| 7:HJ:365:GLY:CA | 7:HJ:392:LEU:HB2 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:117:ILE:HG22 | 5:I:143:TRP:HE3 | 1.79 | 0.47 |
| 8:IB:31:ASN:OD1 | 8:IB:32:PHE:N | 2.48 | 0.47 |
| 11:IE:2:LEU:HD12 | 11:IE:2:LEU:N | 2.30 | 0.47 |
| 12:IF:187:GLY:O | 12:IF:188:LEU:HD12 | 2.14 | 0.47 |
| 5:I:10:VAL:CG1 | 5:K:10:VAL:HG21 | 29.09 | 0.47 |
| 5:K:117:ILE:HG22 | 5:K:143:TRP:CE3 | 2.50 | 0.47 |
| 5:K:396:LYS:O | 5:K:399:ILE:HG13 | 2.14 | 0.47 |
| 5:I:98:VAL:HG11 | 5:K:89:TYR:HB3 | 1.97 | 0.47 |
| 6:L:141:THR:HG22 | 6:N:43:LEU:HD11 | 1.97 | 0.47 |
| 6:M:76:GLY:HA2 | 6:M:215:PHE:HZ | 1.79 | 0.47 |
| 7:P:476:ASP:OD1 | 7:P:479:ASN:ND2 | 2.40 | 0.47 |
| 7:Q:61:PRO:HD3 | 7:Q:74:LYS:HB3 | 1.97 | 0.47 |
| 8:S:14:ASP:CG | 8:S:17:ARG:HH22 | 2.18 | 0.47 |
| 11:V:111:TYR:HB3 | 11:V:121:TYR:HD1 | 1.80 | 0.47 |
| 11:V:132:VAL:HA | 11:V:147:GLU:HA | 1.97 | 0.47 |
| 12:W:23:SER:N | 12:W:202:ASN:O | 2.29 | 0.47 |
| 12:W:21:MET:HB3 | 12:W:204:HIS:O | 2.15 | 0.47 |
| 12:W:223:VAL:HB | 12:W:241:VAL:HG23 | 1.97 | 0.47 |
| 1:X:182:LEU:HD12 | 1:X:182:LEU:O | 2.15 | 0.47 |
| 1:X:472:ASP:C | 1:X:474:SER:H | 2.19 | 0.47 |
| 1:Y:372:ALA:N | 1:Y:404:ILE:HD11 | 2.30 | 0.47 |
| 13:YA:321[A]:LYS:HD3 | 13:YB:452[A]:GLY:CA | 2.34 | 0.47 |
| 13:YA:307[C]:ALA:HB1 | 13:YA:331[C]:ILE:HD11 | 1.96 | 0.47 |
| 13:YA:337[C]:GLU:O | 13:YA:340[C]:GLY:N | 2.48 | 0.47 |
| 13:YA:370[D]:ASN:ND2 | 13:YA:372[D]:SER:HB3 | 2.29 | 0.47 |
| 13:YA:447[F]:ASN:HB3 | 13:YC:376[F]:PHE:CZ | 2.50 | 0.47 |
| 13:YA:450[D]:VAL:O | 13:YC:459[D]:GLY:N | 2.48 | 0.47 |
| 13:YA:567[D]:ILE:HG23 | 13:YB:565[D]:TYR:CE2 | 2.50 | 0.47 |
| 13:YC:189[C]:LYS:HA | 13:YC:234[C]:GLY:O | 2.14 | 0.47 |
| 13:YC:257[C]:LYS:HE2 | 13:YC:266[C]:TRP:CZ2 | 2.50 | 0.47 |
| 13:YC:337[B]:GLU:O | 13:YC:340[B]:GLY:N | 2.48 | 0.47 |
| 13:YB:315[D]:LEU:HD23 | 13:YC:367[D]:PRO:HA | 1.97 | 0.47 |
| 13:YC:387[A]:TYR:CE1 | 13:YC:388[A]:PRO:HB3 | 2.49 | 0.47 |
| 13:YB:481[E]:PHE:O | 13:YC:473[E]:GLN:HA | 2.15 | 0.47 |
| 13:YB:546[A]:VAL:HA | 13:YC:538[A]:VAL:O | 2.14 | 0.47 |
| 13:YB:574[F]:ILE:HG22 | 13:YC:572[F]:ILE:HD13 | 1.97 | 0.47 |
| 13:YA:60[F]:PRO:HD3 | 13:YC:61[F]:ILE:HG12 | 1.97 | 0.47 |
| 14:YD:140[D]:TYR:CD2 | 14:YD:147[D]:THR:HA | 2.50 | 0.47 |
| 14:YD:178[D]:LEU:CD1 | 14:YD:183[D]:ASP:HA | 2.45 | 0.47 |
| 14:YD:212[D]:ILE:HG22 | 14:YD:327[D]:ASN:HB2 | 1.96 | 0.47 |
| 14:YD:244[E]:LYS:O | 14:YD:247[E]:PRO:HD2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:189[F]:TRP:CD1 | 14:YD:320[F]:PRO:HG2 | 2.50 | 0.47 |
| 1:X:287:SER:HB2 | 14:YD:373[B]:LYS:HD2 | 1.97 | 0.47 |
| 14:YD:14[B]:VAL:HG11 | 14:YD:52[B]:LEU:HD11 | 1.96 | 0.47 |
| 14:YD:54[E]:PHE:CZ | 14:YD:105[E]:ILE:HD11 | 2.49 | 0.47 |
| 14:YE:214[E]:GLY:O | 14:YE:215[E]:GLU:HG3 | 2.15 | 0.47 |
| 14:YE:31[B]:LEU:O | 14:YE:35[B]:ILE:HG22 | 2.14 | 0.47 |
| 14:YE:38[E]:LEU:HA | 14:YE:38[E]:LEU:HD12 | 1.63 | 0.47 |
| 14:YF:14[A]:VAL:HG11 | 14:YF:52[A]:LEU:HD11 | 1.96 | 0.47 |
| 14:YF:178[F]:LEU:CD1 | 14:YF:183[F]:ASP:HA | 2.45 | 0.47 |
| 14:YF:189[E]:TRP:CD1 | 14:YF:320[E]:PRO:HG2 | 2.50 | 0.47 |
| 14:YF:189[F]:TRP:CD1 | 14:YF:320[F]:PRO:HG2 | 2.50 | 0.47 |
| 14:YF:212[C]:ILE:HG22 | 14:YF:327[C]:ASN:HB2 | 1.97 | 0.47 |
| 2:Z:177:GLN:HE22 | 2:Z:534:VAL:HG12 | 1.80 | 0.47 |
| 2:Z:712:ASN:HA | 2:Z:751:LEU:HG | 1.97 | 0.47 |
| 1:A:235:GLU:C | 1:A:236:PHE:HD1 | 2.19 | 0.46 |
| 4:AA:202:LEU:HD21 | 4:AA:254:PHE:CZ | 2.50 | 0.46 |
| 4:AB:200:ALA:HB3 | 4:AB:221:ILE:HD11 | 1.96 | 0.46 |
| 5:AE:110:VAL:HG22 | 5:AE:123:PRO:HB3 | 1.97 | 0.46 |
| 7:AJ:415:ASN:O | 7:AJ:424:ARG:HD2 | 2.15 | 0.46 |
| 1:B:209:TRP:NE1 | 1:B:223:ILE:HG12 | 2.30 | 0.46 |
| 1:B:372:ALA:N | 1:B:404:ILE:HD11 | 2.30 | 0.46 |
| 1:B:455:PHE:CD2 | 1:B:456:ASN:N | 2.83 | 0.46 |
| 7:AJ:399:PHE:CD1 | 7:BA:401:ARG:HB3 | 2.50 | 0.46 |
| 7:AJ:429:CYS:SG | 7:BA:515:TRP:NE1 | 2.86 | 0.46 |
| 8:BB:46:VAL:HG13 | 8:BB:63:ASP:O | 2.16 | 0.46 |
| 11:BF:94:TYR:CE1 | 11:BF:156:TYR:HB3 | 2.49 | 0.46 |
| 1:BH:227:ARG:HB2 | 1:BH:237:TYR:CE2 | 2.51 | 0.46 |
| 1:BH:448:TYR:HA | 1:BH:452:VAL:HG12 | 1.95 | 0.46 |
| 1:BI:491:PHE:CE2 | 1:BI:619:GLN:HA | 2.51 | 0.46 |
| 2:BJ:177:GLN:HE22 | 2:BJ:534:VAL:HG12 | 1.80 | 0.46 |
| 2:C:10:SER:O | 2:C:25:TRP:HA | 2.16 | 0.46 |
| 2:C:180:ILE:HG23 | 2:C:201:LEU:HD11 | 1.97 | 0.46 |
| 2:C:340:PRO:HA | 2:C:345:TYR:CD1 | 2.50 | 0.46 |
| 2:C:78:TYR:HB2 | 2:C:100:PHE:CZ | 2.50 | 0.46 |
| 3:CA:177:GLU:HG3 | 3:CA:179:THR:H | 1.80 | 0.46 |
| 4:CC:212:ARG:HG3 | 4:CC:213:LYS:HG3 | 1.96 | 0.46 |
| 4:CC:50:VAL:C | 4:CC:52:ASN:H | 2.17 | 0.46 |
| 5:CF:186:TYR:HE1 | 5:CF:246:THR:HA | 1.80 | 0.46 |
| 5:CF:36:GLU:HA | 5:CF:50:LYS:HZ1 | 1.80 | 0.46 |
| 5:CG:192:ARG:O | 5:CG:244:ILE:HA | 2.15 | 0.46 |
| 3:D:147:LEU:HD23 | 3:D:149:ASP:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:DA:168:LEU:HB2 | 6:DA:180:GLN:OE1 | 2.15 | 0.46 |
| 7:DB:172:LEU:O | 7:DB:175:GLN:HG2 | 2.15 | 0.46 |
| 7:DC:248:ALA:O | 7:DC:252:GLY:N | 2.47 | 0.46 |
| 7:DB:302:ILE:HD12 | 7:DC:306:PHE:CZ | 2.50 | 0.46 |
| 7:DC:359:TRP:CE2 | 7:DC:524:LYS:HD3 | 2.50 | 0.46 |
| 7:DC:85:LEU:O | 7:DC:85:LEU:HD23 | 2.15 | 0.46 |
| 7:DD:221:THR:HG23 | 7:DD:223:GLU:H | 1.80 | 0.46 |
| 7:DD:329:ASN:OD1 | 7:DD:330:ARG:N | 2.48 | 0.46 |
| 8:DF:79:HIS:HE1 | 8:DF:151:GLN:HE22 | 1.63 | 0.46 |
| 10:DH:197:TYR:CZ | 10:GA:290:PRO:HD3 | 2.50 | 0.46 |
| 11:DI:56:PRO:HG3 | 11:DI:86:TRP:NE1 | 2.31 | 0.46 |
| 1:EA:10:LEU:HD11 | 2:EC:701:TRP:HB3 | 1.97 | 0.46 |
| 1:EA:402:ALA:N | 1:EA:403:PRO:HD2 | 2.29 | 0.46 |
| 2:EC:151:PHE:CD2 | 2:EC:166:PHE:HE1 | 2.33 | 0.46 |
| 2:EC:16:LEU:HD23 | 2:EC:102:THR:HA | 1.97 | 0.46 |
| 2:EC:228:ARG:HB3 | 2:EC:250:TYR:HB3 | 1.97 | 0.46 |
| 2:EC:494:GLU:HB2 | 2:EC:498:TRP:HB2 | 1.96 | 0.46 |
| 2:EC:479:TRP:CE2 | 2:EC:505:PRO:HA | 2.50 | 0.46 |
| 2:EC:548:ILE:N | 2:EC:549:PRO:HD3 | 2.30 | 0.46 |
| 2:EC:696:ARG:HH12 | 2:EC:726:PHE:HD1 | 1.63 | 0.46 |
| 3:ED:228:ASN:O | 3:ED:231:TRP:CD1 | 2.69 | 0.46 |
| 4:EF:114:GLY:HA3 | 4:EF:143:TYR:CE2 | 2.49 | 0.46 |
| 5:EI:180:VAL:HG13 | 5:EI:181:PHE:N | 2.29 | 0.46 |
| 5:EJ:169:VAL:O | 5:EJ:238:ILE:HA | 2.15 | 0.46 |
| 5:EJ:250:GLY:N | 5:FA:158:ASP:HB3 | 2.30 | 0.46 |
| 2:EC:221:ALA:H | 5:EJ:562:SER:CB | 2.28 | 0.46 |
| 7:FE:138:SER:C | 7:FG:143:LYS:HG2 | 2.35 | 0.46 |
| 5:AE:362:GLU:CD | 7:FE:473:LYS:HE2 | 2.35 | 0.46 |
| 7:FE:13:SER:CB | 7:FF:18:PHE:HA | 2.40 | 0.46 |
| 7:FF:359:TRP:CE2 | 7:FF:524:LYS:HD3 | 2.50 | 0.46 |
| 7:FF:368:SER:HA | 7:FF:389:ASN:HD22 | 1.79 | 0.46 |
| 8:DE:43:ALA:HB2 | 8:FH:139:GLU:H | 1.80 | 0.46 |
| 10:GA:330:ASN:O | 10:GA:339:PRO:HA | 2.16 | 0.46 |
| 11:GB:132:VAL:HA | 11:GB:147:GLU:HA | 1.97 | 0.46 |
| 12:GC:127:SER:HB3 | 12:GC:161:SER:HG | 1.79 | 0.46 |
| 12:DJ:14:ALA:O | 12:GC:166:SER:HB2 | 2.15 | 0.46 |
| 12:GC:196:GLU:OE2 | 12:GC:217:THR:HG23 | 2.15 | 0.46 |
| 1:GD:145:PHE:HZ | 1:GD:286:PHE:CE1 | 2.32 | 0.46 |
| 1:GD:229:THR:OG1 | 1:GD:233:ASN:OD1 | 2.30 | 0.46 |
| 2:GF:234:SER:HB3 | 2:GF:367:LYS:NZ | 2.29 | 0.46 |
| 3:GG:196:PRO:O | 3:GG:199:SER:HB2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GG:42:GLY:HA2 | 3:GG:76:MET:HG3 | 1.97 | 0.46 |
| 4:GI:8:LYS:HD2 | 4:GI:30:LYS:HA | 1.98 | 0.46 |
| 5:HB:248:MET:HE3 | 5:HC:254:TRP:HB2 | 1.97 | 0.46 |
| 7:O:237:ASN:ND2 | 5:HB:346:GLY:O | 2.34 | 0.46 |
| 2:GF:976:SER:HB2 | 5:HC:10:VAL:HG21 | 1.97 | 0.46 |
| 5:HC:490:TRP:CD1 | 5:HC:516:ALA:HA | 2.49 | 0.46 |
| 5:HD:103:ASN:O | 5:HD:104:VAL:C | 2.54 | 0.46 |
| 5:HD:202:TYR:CZ | 5:HD:225:LEU:HB2 | 2.49 | 0.46 |
| 5:HD:267:ASP:H | 5:HD:377:HIS:HB2 | 1.80 | 0.46 |
| 5:HD:264:ARG:HH22 | 6:HE:2:SER:N | 2.13 | 0.46 |
| 6:HF:54:SER:O | 6:HG:164:GLN:NE2 | 2.48 | 0.46 |
| 6:HG:29:VAL:O | 6:HG:32:ARG:N | 2.36 | 0.46 |
| 7:HH:453:GLU:OE2 | 7:HH:471:THR:N | 2.32 | 0.46 |
| 7:Q:365:GLY:CA | 7:HI:71:ASN:HB2 | 2.40 | 0.46 |
| 7:HI:85:LEU:HD23 | 7:HI:85:LEU:O | 2.15 | 0.46 |
| 7:HJ:325:TYR:CD1 | 7:HJ:330:ARG:HA | 2.45 | 0.46 |
| 5:I:10:VAL:HG23 | 5:I:11:VAL:HG23 | 1.97 | 0.46 |
| 5:I:206:PHE:CD2 | 5:I:223:VAL:HA | 2.50 | 0.46 |
| 5:I:399:ILE:HD12 | 5:K:399:ILE:HG12 | 1.97 | 0.46 |
| 12:GC:215:MET:HE1 | 12:IF:99:SER:HB2 | 1.96 | 0.46 |
| 5:J:170:GLU:O | 5:J:172:GLN:N | 2.48 | 0.46 |
| 5:J:213:GLY:CA | 5:J:221:GLU:HB2 | 2.45 | 0.46 |
| 5:J:192:ARG:O | 5:J:244:ILE:HA | 2.15 | 0.46 |
| 5:J:285:LEU:HD21 | 5:J:375:PHE:N | 2.21 | 0.46 |
| 5:J:490:TRP:CD1 | 5:J:516:ALA:HA | 2.49 | 0.46 |
| 5:K:117:ILE:HG22 | 5:K:143:TRP:HE3 | 1.80 | 0.46 |
| 5:K:289:LYS:HG3 | 5:K:370:HIS:CE1 | 2.50 | 0.46 |
| 5:K:267:ASP:H | 5:K:377:HIS:HB2 | 1.80 | 0.46 |
| 5:J:400:ILE:HG12 | 5:K:402:GLU:OE2 | 2.15 | 0.46 |
| 6:M:125:PHE:O | 6:M:129:VAL:HG23 | 2.14 | 0.46 |
| 7:O:266:THR:HG23 | 7:O:281:LEU:HD23 | 1.97 | 0.46 |
| 7:P:228:ILE:HG21 | 7:P:244:ALA:HB2 | 1.97 | 0.46 |
| 7:Q:335:ASN:OD1 | 7:Q:336:GLU:N | 2.47 | 0.46 |
| 7:O:339:ARG:NH1 | 7:Q:356:SER:HB2 | 2.29 | 0.46 |
| 12:W:214:VAL:HG23 | 12:W:249:GLN:O | 2.15 | 0.46 |
| 1:X:155:ARG:HG2 | 1:X:156:ASP:O | 2.14 | 0.46 |
| 1:X:543:THR:HG23 | 1:X:544:ASP:O | 2.15 | 0.46 |
| 1:Y:37:LEU:HD11 | 1:Y:53:LEU:HD21 | 1.97 | 0.46 |
| 13:YA:39[E]:ARG:NH1 | 13:YA:113[E]:GLY:HA2 | 2.30 | 0.46 |
| 13:YA:393[A]:MET:HA | 13:YC:71[A]:GLY:HA2 | 1.97 | 0.46 |
| 13:YA:461[A]:SER:HA | 13:YC:468[A]:ASP:HB3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:461[C]:SER:HA | 13:YC:468[C]:ASP:HB3 | 1.96 | 0.46 |
| 13:YA:464[F]:TYR:OH | 13:YC:454[F]:LYS:NZ | 2.47 | 0.46 |
| 13:YA:550[A]:TRP:O | 13:YC:558[A]:SER:N | 2.48 | 0.46 |
| 13:YA:567[B]:ILE:HG23 | 13:YB:565[B]:TYR:CE2 | 2.50 | 0.46 |
| 13:YA:567[C]:ILE:HG23 | 13:YB:565[C]:TYR:CE2 | 2.49 | 0.46 |
| 13:YB:81[B]:ARG:HB3 | 13:YB:100[B]:TYR:CZ | 2.50 | 0.46 |
| 13:YB:189[E]:LYS:HA | 13:YB:234[E]:GLY:O | 2.14 | 0.46 |
| 13:YB:257[B]:LYS:HE2 | 13:YB:266[B]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YB:307[C]:ALA:HB1 | 13:YB:331[C]:ILE:HD11 | 1.96 | 0.46 |
| 13:YA:315[A]:LEU:HD23 | 13:YB:367[A]:PRO:HA | 1.97 | 0.46 |
| 13:YB:39[C]:ARG:NH1 | 13:YB:113[C]:GLY:HA2 | 2.30 | 0.46 |
| 13:YB:460[D]:GLY:HA3 | 13:YC:453[D]:ASP:HA | 1.98 | 0.46 |
| 13:YB:540[C]:GLY:HA3 | 13:YC:533[C]:ASN:ND2 | 2.22 | 0.46 |
| 13:YB:81[F]:ARG:HB3 | 13:YB:100[F]:TYR:CZ | 2.51 | 0.46 |
| 13:YA:7[B]:ASN:ND2 | 13:YB:9[B]:ASN:HA | 2.21 | 0.46 |
| 13:YB:315[E]:LEU:HD23 | 13:YC:367[E]:PRO:HA | 1.96 | 0.46 |
| 13:YB:69[C]:ILE:CD1 | 13:YC:396[C]:GLU:HA | 2.45 | 0.46 |
| 13:YB:492[A]:GLY:HA3 | 13:YC:485[A]:ASP:HA | 1.97 | 0.46 |
| 13:YA:34[C]:LEU:HD13 | 14:YD:163[C]:THR:HG21 | 1.96 | 0.46 |
| 14:YD:212[C]:ILE:HG22 | 14:YD:327[C]:ASN:HB2 | 1.97 | 0.46 |
| 14:YD:244[D]:LYS:O | 14:YD:247[D]:PRO:HD2 | 2.14 | 0.46 |
| 14:YD:279[A]:ARG:HD3 | 14:YD:279[A]:ARG:HA | 1.43 | 0.46 |
| 14:YD:31[A]:LEU:O | 14:YD:35[A]:ILE:HG22 | 2.14 | 0.46 |
| 14:YE:10[D]:PRO:HD2 | 14:YE:349[D]:ASN:O | 2.15 | 0.46 |
| 14:YE:178[B]:LEU:CD1 | 14:YE:183[B]:ASP:HA | 2.45 | 0.46 |
| 14:YE:214[F]:GLY:O | 14:YE:215[F]:GLU:HG3 | 2.14 | 0.46 |
| 11:DI:178:ASN:HB3 | 14:YE:217[B]:SER:H | 1.80 | 0.46 |
| 14:YE:244[B]:LYS:O | 14:YE:247[B]:PRO:HD2 | 2.14 | 0.46 |
| 14:YE:332[B]:GLN:HB3 | 14:YF:61[B]:HIS:NE2 | 2.30 | 0.46 |
| 14:YE:336[A]:GLU:O | 14:YE:359[A]:THR:OG1 | 2.33 | 0.46 |
| 14:YF:15[C]:LYS:HB3 | 14:YF:15[C]:LYS:HE2 | 1.53 | 0.46 |
| 14:YF:185[B]:PHE:CD2 | 14:YF:297[B]:ARG:HA | 2.49 | 0.46 |
| 14:YF:212[B]:ILE:HG22 | 14:YF:327[B]:ASN:HB2 | 1.97 | 0.46 |
| 14:YF:214[C]:GLY:O | 14:YF:215[C]:GLU:HG3 | 2.14 | 0.46 |
| 11:IE:178:ASN:HB3 | 14:YF:217[B]:SER:H | 1.80 | 0.46 |
| 14:YF:244[F]:LYS:O | 14:YF:247[F]:PRO:HD2 | 2.14 | 0.46 |
| 14:YF:336[A]:GLU:O | 14:YF:359[A]:THR:OG1 | 2.33 | 0.46 |
| 2:Z:228:ARG:HB3 | 2:Z:250:TYR:HB3 | 1.97 | 0.46 |
| 2:Z:10:SER:O | 2:Z:25:TRP:HA | 2.16 | 0.46 |
| 2:Z:91:GLN:HE21 | 2:Z:92:SER:H | 1.62 | 0.46 |
| 1:A:182:LEU:HD12 | 1:A:182:LEU:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:444:ILE:O | 1:A:447:TYR:HB3 | 2.15 | 0.46 |
| 5:AC:496:ASP:OD2 | 5:AC:499:PHE:HB2 | 2.15 | 0.46 |
| 5:AD:130:PHE:HB2 | 5:AD:150:GLN:HB3 | 1.98 | 0.46 |
| 6:AF:74:LYS:HG3 | 6:AH:70:ILE:HD11 | 1.97 | 0.46 |
| 6:AG:76:GLY:HA2 | 6:AG:215:PHE:HZ | 1.80 | 0.46 |
| 6:AH:90:PHE:CD2 | 6:AH:126:VAL:HG22 | 2.45 | 0.46 |
| 7:AI:110:VAL:HG12 | 7:AI:111:ASN:N | 2.30 | 0.46 |
| 7:AI:12:GLU:HG3 | 7:AI:14:ARG:N | 2.31 | 0.46 |
| 7:AI:493:GLU:HG3 | 7:AI:496:ARG:HH21 | 1.80 | 0.46 |
| 1:B:424:TYR:HE2 | 1:B:655:LEU:HD13 | 1.81 | 0.46 |
| 7:AI:329:ASN:CG | 7:BA:333:THR:HB | 2.34 | 0.46 |
| 8:BC:31:ASN:OD1 | 8:BC:32:PHE:N | 2.48 | 0.46 |
| 8:BC:46:VAL:HG13 | 8:BC:63:ASP:O | 2.16 | 0.46 |
| 11:BF:111:TYR:HB3 | 11:BF:121:TYR:HD1 | 1.80 | 0.46 |
| 1:BH:102:SER:OG | 1:BH:103:LYS:N | 2.48 | 0.46 |
| 1:BH:210:THR:HG22 | 1:BH:226:MET:H | 1.79 | 0.46 |
| 1:BH:565:GLU:HB3 | 1:BH:570:GLN:OE1 | 2.16 | 0.46 |
| 1:BH:595:ILE:HG22 | 1:BH:602:ILE:HA | 1.98 | 0.46 |
| 2:BJ:479:TRP:CE2 | 2:BJ:505:PRO:HA | 2.50 | 0.46 |
| 2:BJ:645:LEU:HD11 | 11:DI:83:TYR:CD1 | 2.51 | 0.46 |
| 2:BJ:91:GLN:HE21 | 2:BJ:92:SER:H | 1.62 | 0.46 |
| 2:BJ:934:ALA:H | 2:BJ:997:SER:HB2 | 1.79 | 0.46 |
| 2:C:777:LEU:HD12 | 2:C:778:THR:H | 1.79 | 0.46 |
| 3:CA:131:TYR:CE1 | 3:CA:190:TYR:HD1 | 2.33 | 0.46 |
| 2:BJ:58:ASN:HB3 | 4:CD:155:ASN:ND2 | 2.31 | 0.46 |
| 5:CG:116:THR:HA | 5:CG:121:ALA:HB2 | 1.96 | 0.46 |
| 5:CG:170:GLU:O | 5:CG:172:GLN:N | 2.48 | 0.46 |
| 5:CG:313:PHE:HE2 | 5:CG:320:LEU:HD11 | 1.80 | 0.46 |
| 5:CG:358:VAL:HG23 | 5:CG:371:PHE:HD1 | 1.80 | 0.46 |
| 5:CG:400:ILE:HG12 | 5:CH:402:GLU:OE2 | 2.15 | 0.46 |
| 5:CH:326:MET:HE3 | 5:CH:326:MET:HB2 | 1.78 | 0.46 |
| 6:CJ:168:LEU:HB2 | 6:CJ:180:GLN:OE1 | 2.15 | 0.46 |
| 3:D:228:ASN:O | 3:D:231:TRP:CD1 | 2.69 | 0.46 |
| 3:D:233:GLN:HB2 | 3:E:289:ASN:HD21 | 1.79 | 0.46 |
| 6:DA:76:GLY:HA2 | 6:DA:215:PHE:HZ | 1.79 | 0.46 |
| 7:DB:255:SER:O | 7:DB:278:SER:OG | 2.29 | 0.46 |
| 7:DD:167:GLN:HG3 | 7:DD:168:LEU:HG | 1.98 | 0.46 |
| 7:DB:329:ASN:HD21 | 7:DD:335:ASN:H | 1.63 | 0.46 |
| 8:DE:79:HIS:CE1 | 8:DE:151:GLN:HE22 | 2.33 | 0.46 |
| 8:DF:69:TRP:CZ3 | 8:DF:157:LEU:HD12 | 2.51 | 0.46 |
| 1:BI:76:TYR:CE2 | 11:DI:31:ASN:HA | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:643:PRO:HG2 | 11:DI:84:TYR:CE2 | 2.50 | 0.46 |
| 3:E:219:ASP:CG | 3:E:222:ARG:H | 2.19 | 0.46 |
| 3:E:29:GLY:HA2 | 3:E:34:LYS:HE3 | 1.96 | 0.46 |
| 1:EA:210:THR:HG22 | 1:EA:225:TYR:HA | 1.95 | 0.46 |
| 1:EA:634:THR:HB | 1:EA:638:SER:O | 2.14 | 0.46 |
| 1:EB:491:PHE:CE2 | 1:EB:619:GLN:HA | 2.51 | 0.46 |
| 2:EC:189:ARG:HD3 | 2:EC:203:GLU:OE2 | 2.14 | 0.46 |
| 2:EC:562:ASP:O | 2:EC:565:ASP:N | 2.44 | 0.46 |
| 2:EC:613:LYS:O | 2:EC:615:THR:N | 2.47 | 0.46 |
| 2:EC:664:PHE:O | 2:EC:667:PHE:HB3 | 2.15 | 0.46 |
| 2:EC:91:GLN:HE21 | 2:EC:92:SER:H | 1.62 | 0.46 |
| 3:ED:104:TYR:HE2 | 3:ED:165:ARG:HH21 | 1.63 | 0.46 |
| 3:EE:219:ASP:CG | 3:EE:222:ARG:H | 2.19 | 0.46 |
| 4:EG:178:THR:HA | 4:EG:275:ALA:HA | 1.97 | 0.46 |
| 5:EJ:313:PHE:HE2 | 5:EJ:320:LEU:HD11 | 1.80 | 0.46 |
| 5:EJ:360:THR:HG22 | 5:EJ:366:PRO:HG3 | 1.96 | 0.46 |
| 4:F:212:ARG:HG3 | 4:F:213:LYS:HG3 | 1.96 | 0.46 |
| 4:F:178:THR:HA | 4:F:275:ALA:HA | 1.97 | 0.46 |
| 5:FA:117:ILE:HG22 | 5:FA:143:TRP:HE3 | 1.80 | 0.46 |
| 5:FA:358:VAL:HA | 5:FA:371:PHE:HA | 1.96 | 0.46 |
| 5:EJ:2:LYS:H | 5:FA:41:ASP:HB3 | 1.80 | 0.46 |
| 7:FE:39:ILE:HD13 | 7:FG:39:ILE:HD13 | 1.96 | 0.46 |
| 7:FF:227:VAL:HG23 | 7:FG:225:LYS:HD3 | 1.96 | 0.46 |
| 7:FG:160:MET:HG2 | 7:FG:165:THR:HB | 1.96 | 0.46 |
| 11:GB:94:TYR:CE1 | 11:GB:156:TYR:HB3 | 2.49 | 0.46 |
| 1:GE:175:THR:O | 1:GE:270:ILE:HG22 | 2.15 | 0.46 |
| 2:GF:1003:GLN:OE1 | 5:HB:10:VAL:HA | 2.16 | 0.46 |
| 2:GF:78:TYR:HB2 | 2:GF:100:PHE:CZ | 2.50 | 0.46 |
| 2:GF:196:GLU:HG2 | 2:GF:197:GLY:N | 2.29 | 0.46 |
| 2:GF:406:LEU:CD1 | 2:GF:413:TRP:HA | 2.44 | 0.46 |
| 2:GF:698:GLU:HG3 | 2:GF:699:HIS:N | 2.30 | 0.46 |
| 2:GF:777:LEU:HD12 | 2:GF:778:THR:N | 2.30 | 0.46 |
| 3:GG:228:ASN:O | 3:GG:231:TRP:CD1 | 2.69 | 0.46 |
| 2:EC:484:HIS:ND1 | 3:GH:232:GLN:OE1 | 2.32 | 0.46 |
| 3:GH:248:ARG:HA | 3:GH:331:LEU:HD23 | 1.97 | 0.46 |
| 4:GJ:212:ARG:HG3 | 4:GJ:213:LYS:HG3 | 1.96 | 0.46 |
| 4:GJ:202:LEU:HD21 | 4:GJ:254:PHE:CZ | 2.50 | 0.46 |
| 4:HA:178:THR:HA | 4:HA:275:ALA:HA | 1.97 | 0.46 |
| 5:HB:186:TYR:HE1 | 5:HB:246:THR:HA | 1.80 | 0.46 |
| 5:HB:313:PHE:HE2 | 5:HB:320:LEU:HD11 | 1.80 | 0.46 |
| 5:HB:558:ASP:N | 5:HB:559:PRO:HD3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:103:ASN:CG | 5:HC:104:VAL:H | 2.17 | 0.46 |
| 5:HC:130:PHE:HB2 | 5:HC:150:GLN:HB3 | 1.98 | 0.46 |
| 5:HD:117:ILE:HG22 | 5:HD:143:TRP:CE3 | 2.50 | 0.46 |
| 5:HD:86:VAL:HG13 | 5:HD:87:ASN:N | 2.29 | 0.46 |
| 6:HE:125:PHE:O | 6:HE:129:VAL:HG23 | 2.14 | 0.46 |
| 6:HE:13:ARG:HG2 | 6:HE:14:LEU:N | 2.27 | 0.46 |
| 7:HH:357:ASP:OD1 | 7:HI:339:ARG:NH2 | 2.48 | 0.46 |
| 7:HH:95:TYR:HA | 7:HJ:98:THR:O | 2.15 | 0.46 |
| 7:HI:29:ILE:O | 7:HI:30:THR:OG1 | 2.24 | 0.46 |
| 7:HH:138:SER:C | 7:HJ:143:LYS:HG2 | 2.35 | 0.46 |
| 11:IE:56:PRO:HG3 | 11:IE:86:TRP:NE1 | 2.31 | 0.46 |
| 5:J:48:ALA:O | 5:J:49:TRP:HD1 | 1.97 | 0.46 |
| 5:J:542:LEU:HD21 | 5:K:569:TYR:OH | 2.15 | 0.46 |
| 5:J:567:THR:O | 5:K:551:ILE:HA | 2.15 | 0.46 |
| 5:K:275:SER:OG | 5:K:282:VAL:HG12 | 2.16 | 0.46 |
| 7:O:12:GLU:HG3 | 7:O:15:TYR:H | 1.79 | 0.46 |
| 7:P:415:ASN:O | 7:P:424:ARG:HD2 | 2.15 | 0.46 |
| 7:P:141:VAL:HG22 | 7:Q:139:ASN:HB2 | 1.96 | 0.46 |
| 7:O:39:ILE:HA | 7:Q:44:VAL:HG22 | 1.97 | 0.46 |
| 8:R:46:VAL:HG13 | 8:R:63:ASP:O | 2.16 | 0.46 |
| 10:U:203:ARG:NH2 | 10:U:356:ARG:HH12 | 2.13 | 0.46 |
| 10:U:218:ASP:OD2 | 12:IF:143:TYR:OH | 2.24 | 0.46 |
| 10:U:334:ILE:HG13 | 10:U:335:ALA:N | 2.30 | 0.46 |
| 12:W:31:SER:O | 12:W:32:THR:OG1 | 2.30 | 0.46 |
| 1:X:634:THR:HB | 1:X:638:SER:O | 2.14 | 0.46 |
| 1:Y:143:TYR:CD2 | 1:Y:279:ASP:HB2 | 2.50 | 0.46 |
| 13:YA:146[A]:VAL:O | 13:YA:150[A]:SER:OG | 2.34 | 0.46 |
| 13:YA:189[C]:LYS:HA | 13:YA:234[C]:GLY:O | 2.14 | 0.46 |
| 13:YA:337[F]:GLU:O | 13:YA:340[F]:GLY:N | 2.48 | 0.46 |
| 13:YA:60[F]:PRO:HB3 | 13:YC:60[F]:PRO:HB3 | 1.97 | 0.46 |
| 13:YA:18[F]:ARG:CZ | 13:YA:77[F]:VAL:HG23 | 2.45 | 0.46 |
| 13:YB:81[A]:ARG:HB3 | 13:YB:100[A]:TYR:CZ | 2.51 | 0.46 |
| 13:YB:121[E]:TYR:OH | 13:YB:123[E]:ARG:NH2 | 2.48 | 0.46 |
| 13:YB:257[E]:LYS:HE2 | 13:YB:266[E]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YC:81[A]:ARG:HB3 | 13:YC:100[A]:TYR:CZ | 2.51 | 0.46 |
| 13:YC:146[D]:VAL:O | 13:YC:150[D]:SER:OG | 2.34 | 0.46 |
| 13:YC:337[C]:GLU:O | 13:YC:340[C]:GLY:N | 2.48 | 0.46 |
| 13:YB:315[B]:LEU:HD23 | 13:YC:367[B]:PRO:HA | 1.96 | 0.46 |
| 13:YC:370[C]:ASN:ND2 | 13:YC:372[C]:SER:HB3 | 2.29 | 0.46 |
| 13:YA:564[A]:GLN:HE22 | 13:YC:571[A]:ARG:HD3 | 1.79 | 0.46 |
| 13:YA:121[A]:TYR:HB3 | 13:YC:66[A]:MET:SD | 2.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:123[B]:ARG:HB2 | 13:YC:67[B]:SER:HB3 | 1.96 | 0.46 |
| 14:YD:140[E]:TYR:CD2 | 14:YD:147[E]:THR:HA | 2.50 | 0.46 |
| 14:YD:178[C]:LEU:CD1 | 14:YD:183[C]:ASP:HA | 2.45 | 0.46 |
| 14:YD:31[D]:LEU:O | 14:YD:35[D]:ILE:HG22 | 2.14 | 0.46 |
| 14:YE:14[A]:VAL:HG11 | 14:YE:52[A]:LEU:HD11 | 1.96 | 0.46 |
| 14:YE:178[A]:LEU:CD1 | 14:YE:183[A]:ASP:HA | 2.45 | 0.46 |
| 14:YE:185[D]:PHE:CD2 | 14:YE:297[D]:ARG:HA | 2.49 | 0.46 |
| 14:YE:236[A]:TRP:N | 14:YF:95[A]:VAL:O | 2.48 | 0.46 |
| 14:YE:10[F]:PRO:HD2 | 14:YE:349[F]:ASN:O | 2.16 | 0.46 |
| 14:YE:14[E]:VAL:HG11 | 14:YE:52[E]:LEU:HD11 | 1.96 | 0.46 |
| 14:YE:70[F]:ILE:N | 14:YE:88[F]:TYR:O | 2.49 | 0.46 |
| 14:YD:332[E]:GLN:NE2 | 14:YE:97[E]:VAL:HG21 | 2.30 | 0.46 |
| 14:YF:140[F]:TYR:CD2 | 14:YF:147[F]:THR:HA | 2.50 | 0.46 |
| 14:YF:178[E]:LEU:CD1 | 14:YF:183[E]:ASP:HA | 2.45 | 0.46 |
| 14:YF:212[E]:ILE:HG22 | 14:YF:327[E]:ASN:HB2 | 1.97 | 0.46 |
| 2:Z:180:ILE:HG23 | 2:Z:201:LEU:HD11 | 1.97 | 0.46 |
| 2:Z:193:MET:HB3 | 2:Z:200:TYR:HB2 | 1.98 | 0.46 |
| 2:Z:193:MET:N | 2:Z:200:TYR:O | 2.37 | 0.46 |
| 2:Z:777:LEU:HD12 | 2:Z:778:THR:N | 2.30 | 0.46 |
| 1:A:174:ARG:HH21 | 1:A:269:VAL:HG21 | 1.80 | 0.46 |
| 5:AC:186:TYR:HB3 | 5:AC:227:GLY:O | 2.14 | 0.46 |
| 5:AC:248:MET:HE3 | 5:AD:254:TRP:HB2 | 1.96 | 0.46 |
| 5:AC:23:GLY:O | 5:AC:24:ILE:HB | 2.15 | 0.46 |
| 5:AC:316:ILE:HG22 | 5:AC:318:GLN:HG3 | 1.96 | 0.46 |
| 5:AD:189:ASN:HD21 | 5:AE:150:GLN:HE22 | 1.63 | 0.46 |
| 5:AD:290:SER:CB | 5:AD:371:PHE:H | 2.27 | 0.46 |
| 5:AD:3:GLN:HG3 | 5:AD:25:LYS:HG3 | 1.98 | 0.46 |
| 5:AD:506:LEU:HD23 | 5:AD:512:PRO:HA | 1.96 | 0.46 |
| 5:AE:117:ILE:HG22 | 5:AE:143:TRP:CE3 | 2.50 | 0.46 |
| 7:AI:263:VAL:O | 7:AJ:260:ARG:HA | 2.14 | 0.46 |
| 1:B:179:TYR:HD1 | 1:B:185:ILE:HD11 | 1.79 | 0.46 |
| 1:B:377:LYS:HB3 | 1:B:377:LYS:HE2 | 1.65 | 0.46 |
| 7:AJ:227:VAL:HG23 | 7:BA:225:LYS:HB3 | 1.98 | 0.46 |
| 7:AI:469:VAL:HB | 7:BA:477:TRP:CZ3 | 2.51 | 0.46 |
| 12:BG:223:VAL:HB | 12:BG:241:VAL:HG23 | 1.97 | 0.46 |
| 1:BI:209:TRP:NE1 | 1:BI:223:ILE:HG12 | 2.30 | 0.46 |
| 2:BJ:180:ILE:HG23 | 2:BJ:201:LEU:HD11 | 1.97 | 0.46 |
| 2:BJ:938:PRO:HD2 | 2:BJ:943:GLU:HB2 | 1.97 | 0.46 |
| 2:C:193:MET:N | 2:C:200:TYR:O | 2.37 | 0.46 |
| 2:C:328:TYR:H | 2:C:353:ASP:CG | 2.19 | 0.46 |
| 2:C:696:ARG:HH12 | 2:C:726:PHE:HD1 | 1.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:821:ILE:O | 2:C:824:GLN:NE2 | 2.32 | 0.46 |
| 3:CA:104:TYR:HE2 | 3:CA:165:ARG:HH21 | 1.63 | 0.46 |
| 3:CA:174:GLY:HA3 | 3:CA:180:ILE:HG12 | 1.97 | 0.46 |
| 4:CC:172:GLU:OE1 | 4:CD:164:ILE:HG23 | 2.14 | 0.46 |
| 4:CC:83:THR:HA | 4:CE:63:ALA:HB3 | 1.96 | 0.46 |
| 5:CF:182:ARG:HH22 | 5:CG:299:ILE:HG21 | 1.80 | 0.46 |
| 5:CF:183:GLY:HA2 | 5:CF:307:ASN:ND2 | 2.31 | 0.46 |
| 5:CF:584:THR:O | 5:CG:531:ASN:ND2 | 2.44 | 0.46 |
| 5:CG:359:GLU:H | 5:CG:370:HIS:C | 2.16 | 0.46 |
| 5:CG:477:SER:HB2 | 5:CG:602:ALA:HB3 | 1.96 | 0.46 |
| 5:CH:103:ASN:O | 5:CH:104:VAL:C | 2.54 | 0.46 |
| 5:CH:117:ILE:HG22 | 5:CH:143:TRP:CE3 | 2.50 | 0.46 |
| 6:CI:168:LEU:HB2 | 6:CI:180:GLN:OE1 | 2.15 | 0.46 |
| 7:DB:329:ASN:CG | 7:DD:333:THR:HB | 2.35 | 0.46 |
| 7:DB:349:TRP:NE1 | 7:DB:351:ALA:HB3 | 2.30 | 0.46 |
| 7:DB:447:HIS:CE1 | 7:DD:445:HIS:NE2 | 2.82 | 0.46 |
| 7:DC:118:PRO:HG3 | 7:DD:106:ALA:HA | 1.96 | 0.46 |
| 7:DD:168:LEU:HD23 | 7:DD:168:LEU:HA | 1.79 | 0.46 |
| 7:DB:471:THR:HA | 7:DD:474:GLY:O | 2.14 | 0.46 |
| 11:DI:175:SER:HA | 14:YF:217[F]:SER:HB2 | 1.96 | 0.46 |
| 1:BI:76:TYR:CE1 | 11:DI:31:ASN:HB3 | 2.51 | 0.46 |
| 1:EA:145:PHE:HZ | 1:EA:286:PHE:CE1 | 2.32 | 0.46 |
| 1:EA:595:ILE:HG22 | 1:EA:602:ILE:HA | 1.97 | 0.46 |
| 1:EB:23:GLY:O | 1:EB:29:ILE:HD11 | 2.15 | 0.46 |
| 1:EB:175:THR:O | 1:EB:270:ILE:HG22 | 2.15 | 0.46 |
| 1:EB:502:ASN:OD1 | 1:EB:635:ARG:NH2 | 2.48 | 0.46 |
| 2:EC:569:VAL:HB | 2:EC:617:VAL:HG12 | 1.98 | 0.46 |
| 2:EC:604:VAL:HG22 | 2:EC:605:ARG:H | 1.80 | 0.46 |
| 2:EC:712:ASN:HA | 2:EC:751:LEU:HG | 1.97 | 0.46 |
| 3:ED:196:PRO:O | 3:ED:199:SER:HB2 | 2.14 | 0.46 |
| 4:EH:85:HIS:HD2 | 4:EH:109:PHE:HE1 | 1.62 | 0.46 |
| 5:EI:139:ALA:O | 5:EI:141:GLY:N | 2.47 | 0.46 |
| 5:EI:206:PHE:CD2 | 5:EI:223:VAL:HA | 2.50 | 0.46 |
| 5:EI:240:ASP:HA | 7:FE:5:THR:OG1 | 2.16 | 0.46 |
| 5:EI:183:GLY:HA2 | 5:EI:307:ASN:ND2 | 2.31 | 0.46 |
| 5:EI:45:SER:OG | 5:FA:66:LYS:HA | 2.15 | 0.46 |
| 4:F:67:TYR:CD1 | 4:F:84:ARG:HB3 | 2.50 | 0.46 |
| 5:FA:264:ARG:HH22 | 6:FB:2:SER:N | 2.13 | 0.46 |
| 6:FB:71:ILE:O | 6:FB:215:PHE:N | 2.36 | 0.46 |
| 6:FC:168:LEU:HB2 | 6:FC:180:GLN:OE1 | 2.15 | 0.46 |
| 7:FF:117:THR:CB | 7:FG:112:ASN:HA | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:515:TRP:HE1 | 7:FG:429:CYS:HG | 1.63 | 0.46 |
| 8:FI:79:HIS:HE1 | 8:FI:151:GLN:HE22 | 1.63 | 0.46 |
| 10:GA:334:ILE:HG13 | 10:GA:335:ALA:N | 2.29 | 0.46 |
| 11:GB:56:PRO:HG3 | 11:GB:86:TRP:NE1 | 2.31 | 0.46 |
| 12:GC:223:VAL:HB | 12:GC:241:VAL:HG23 | 1.97 | 0.46 |
| 1:GD:227:ARG:HB2 | 1:GD:237:TYR:CE2 | 2.51 | 0.46 |
| 1:GD:345:TYR:OH | 1:GD:400:ASN:CG | 2.54 | 0.46 |
| 1:GE:372:ALA:N | 1:GE:404:ILE:HD11 | 2.30 | 0.46 |
| 1:GE:363:PHE:CG | 1:GE:636:ASP:HB2 | 2.50 | 0.46 |
| 2:GF:525:TRP:NE1 | 2:GF:526:ILE:O | 2.49 | 0.46 |
| 3:GH:196:PRO:O | 3:GH:199:SER:OG | 2.25 | 0.46 |
| 3:GH:40:THR:O | 3:GH:273:SER:N | 2.44 | 0.46 |
| 4:GI:212:ARG:HG3 | 4:GI:213:LYS:HG3 | 1.96 | 0.46 |
| 4:GI:202:LEU:HD21 | 4:GI:254:PHE:CZ | 2.50 | 0.46 |
| 4:H:212:ARG:HG3 | 4:H:213:LYS:HG3 | 1.96 | 0.46 |
| 5:HB:194:LYS:HB3 | 5:HB:196:ARG:H | 1.78 | 0.46 |
| 5:HC:192:ARG:O | 5:HC:244:ILE:HA | 2.15 | 0.46 |
| 5:HC:97:ASP:OD1 | 5:HC:102:TRP:CE2 | 2.68 | 0.46 |
| 5:HD:356:TYR:CE1 | 6:HF:4:LEU:HD13 | 2.51 | 0.46 |
| 5:HD:289:LYS:HG3 | 5:HD:370:HIS:CE1 | 2.50 | 0.46 |
| 6:HE:10:VAL:HG11 | 6:HG:10:VAL:HG21 | 1.98 | 0.46 |
| 6:HE:13:ARG:NH1 | 6:HG:47:PHE:CE1 | 2.84 | 0.46 |
| 6:HF:125:PHE:O | 6:HF:129:VAL:HG23 | 2.14 | 0.46 |
| 7:HH:110:VAL:HG12 | 7:HH:111:ASN:N | 2.30 | 0.46 |
| 7:HH:349:TRP:NE1 | 7:HH:351:ALA:HB3 | 2.30 | 0.46 |
| 7:HH:371:ASP:OD1 | 7:HH:526:LYS:NZ | 2.47 | 0.46 |
| 7:HI:228:ILE:HG21 | 7:HI:244:ALA:HB2 | 1.97 | 0.46 |
| 7:HH:513:ARG:N | 7:HI:441:GLN:O | 2.34 | 0.46 |
| 7:HI:335:ASN:H | 7:HJ:329:ASN:HD21 | 1.64 | 0.46 |
| 7:HI:348:MET:SD | 7:HJ:400:VAL:HG11 | 2.56 | 0.46 |
| 7:HH:504:ARG:NH2 | 7:HJ:424:ARG:O | 2.47 | 0.46 |
| 5:I:318:GLN:HB3 | 6:N:4:LEU:CD1 | 2.46 | 0.46 |
| 8:IB:14:ASP:CG | 8:IB:17:ARG:HH22 | 2.18 | 0.46 |
| 8:IB:46:VAL:HG13 | 8:IB:63:ASP:O | 2.16 | 0.46 |
| 5:J:120:SER:OG | 5:J:122:VAL:HG22 | 2.16 | 0.46 |
| 5:J:265:LEU:HG | 5:J:379:ASP:HB2 | 1.98 | 0.46 |
| 6:L:100:PRO:O | 6:L:103:SER:OG | 2.18 | 0.46 |
| 7:Q:375:TYR:CZ | 7:Q:392:LEU:HD23 | 2.50 | 0.46 |
| 7:Q:7:GLN:HB3 | 7:Q:15:TYR:CE2 | 2.51 | 0.46 |
| 8:S:31:ASN:OD1 | 8:S:32:PHE:N | 2.48 | 0.46 |
| 8:S:46:VAL:HG13 | 8:S:63:ASP:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:S:69:TRP:CZ3 | 8:S:157:LEU:HD12 | 2.51 | 0.46 |
| 10:U:330:ASN:O | 10:U:339:PRO:HA | 2.16 | 0.46 |
| 11:V:2:LEU:HD12 | 11:V:2:LEU:N | 2.30 | 0.46 |
| 1:X:179:TYR:HD1 | 1:X:185:ILE:HD11 | 1.80 | 0.46 |
| 1:X:508:ARG:HH22 | 1:X:577:PHE:CA | 2.27 | 0.46 |
| 1:Y:175:THR:O | 1:Y:270:ILE:HG22 | 2.15 | 0.46 |
| 1:Y:356:ILE:HG21 | 1:Y:388:GLN:NE2 | 2.30 | 0.46 |
| 1:Y:514:THR:HG22 | 1:Y:539:ARG:HB2 | 1.96 | 0.46 |
| 13:YA:148[B]:GLN:NE2 | 13:YA:421[B]:TYR:OH | 2.48 | 0.46 |
| 13:YA:337[A]:GLU:O | 13:YA:340[A]:GLY:N | 2.48 | 0.46 |
| 13:YA:39[F]:ARG:NH1 | 13:YA:113[F]:GLY:HA2 | 2.30 | 0.46 |
| 13:YA:447[D]:ASN:HB3 | 13:YC:376[D]:PHE:CZ | 2.50 | 0.46 |
| 13:YB:39[A]:ARG:NH1 | 13:YB:113[A]:GLY:HA2 | 2.30 | 0.46 |
| 13:YB:148[E]:GLN:NE2 | 13:YB:421[E]:TYR:OH | 2.48 | 0.46 |
| 13:YB:257[F]:LYS:HE2 | 13:YB:266[F]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YA:70[E]:GLY:O | 13:YB:394[E]:GLU:N | 2.48 | 0.46 |
| 13:YC:81[D]:ARG:HB3 | 13:YC:100[D]:TYR:CZ | 2.51 | 0.46 |
| 13:YC:180[B]:LEU:HD13 | 13:YC:180[B]:LEU:HA | 1.76 | 0.46 |
| 13:YB:561[E]:SER:HA | 13:YC:554[E]:MET:O | 2.16 | 0.46 |
| 13:YA:550[D]:TRP:O | 13:YC:558[D]:SER:N | 2.48 | 0.46 |
| 13:YB:574[B]:ILE:HG22 | 13:YC:572[B]:ILE:HD13 | 1.97 | 0.46 |
| 13:YA:122[A]:PRO:HB3 | 13:YC:66[A]:MET:HE2 | 1.96 | 0.46 |
| 13:YC:81[B]:ARG:HB3 | 13:YC:100[B]:TYR:CZ | 2.50 | 0.46 |
| 14:YD:14[A]:VAL:HG11 | 14:YD:52[A]:LEU:HD11 | 1.96 | 0.46 |
| 14:YD:236[C]:TRP:N | 14:YE:95[C]:VAL:O | 2.49 | 0.46 |
| 14:YD:307[B]:TYR:HD1 | 14:YD:307[B]:TYR:HA | 1.66 | 0.46 |
| 14:YD:336[A]:GLU:O | 14:YD:359[A]:THR:OG1 | 2.33 | 0.46 |
| 14:YD:70[F]:ILE:N | 14:YD:88[F]:TYR:O | 2.49 | 0.46 |
| 14:YE:140[D]:TYR:CD2 | 14:YE:147[D]:THR:HA | 2.50 | 0.46 |
| 14:YE:140[B]:TYR:CD2 | 14:YE:147[B]:THR:HA | 2.50 | 0.46 |
| 14:YE:14[C]:VAL:HG11 | 14:YE:52[C]:LEU:HD11 | 1.97 | 0.46 |
| 14:YE:279[E]:ARG:HD3 | 14:YE:279[E]:ARG:HA | 1.43 | 0.46 |
| 14:YF:109[E]:LEU:HA | 14:YF:109[E]:LEU:HD12 | 1.65 | 0.46 |
| 14:YE:234[F]:PHE:HD1 | 14:YF:97[F]:VAL:HG12 | 1.80 | 0.46 |
| 2:Z:525:TRP:CE2 | 2:Z:526:ILE:O | 2.68 | 0.46 |
| 2:Z:853:ASP:OD1 | 2:Z:854:TYR:N | 2.47 | 0.46 |
| 1:A:52:ARG:NH2 | 9:T:25:ARG:HB3 | 2.31 | 0.46 |
| 1:A:554:ILE:HG22 | 1:A:555:ILE:O | 2.16 | 0.46 |
| 4:AA:53:GLY:HA3 | 4:AB:7:LYS:HE2 | 1.97 | 0.46 |
| 5:AC:183:GLY:HA2 | 5:AC:307:ASN:ND2 | 2.31 | 0.46 |
| 5:AD:265:LEU:HG | 5:AD:379:ASP:HB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:104:VAL:HG13 | 5:AE:105:ASN:H | 1.80 | 0.46 |
| 5:AE:344:VAL:O | 5:AE:345:LEU:HD12 | 2.16 | 0.46 |
| 5:AE:358:VAL:HG22 | 5:AE:371:PHE:HB2 | 1.98 | 0.46 |
| 6:AG:168:LEU:HB2 | 6:AG:180:GLN:OE1 | 2.15 | 0.46 |
| 7:AI:172:LEU:O | 7:AI:175:GLN:HG2 | 2.15 | 0.46 |
| 7:AI:95:TYR:HA | 7:BA:98:THR:O | 2.14 | 0.46 |
| 1:B:143:TYR:CD2 | 1:B:279:ASP:HB2 | 2.49 | 0.46 |
| 1:B:351:GLU:N | 1:B:351:GLU:OE1 | 2.48 | 0.46 |
| 1:B:356:ILE:HG21 | 1:B:388:GLN:NE2 | 2.30 | 0.46 |
| 1:B:502:ASN:OD1 | 1:B:635:ARG:NH2 | 2.48 | 0.46 |
| 1:B:572:TYR:HB2 | 1:B:591:VAL:HG23 | 1.97 | 0.46 |
| 7:BA:221:THR:HG23 | 7:BA:223:GLU:H | 1.80 | 0.46 |
| 7:AJ:335:ASN:H | 7:BA:329:ASN:HD21 | 1.63 | 0.46 |
| 7:BA:7:GLN:HB3 | 7:BA:15:TYR:CE2 | 2.51 | 0.46 |
| 5:AD:196:ARG:HH22 | 7:BA:9:VAL:HG12 | 1.81 | 0.46 |
| 8:R:55:ASN:HD22 | 8:BB:99:ILE:HD11 | 1.81 | 0.46 |
| 8:BC:114:ARG:HD2 | 8:BC:123:VAL:HG11 | 1.97 | 0.46 |
| 8:BC:40:ALA:O | 8:BC:69:TRP:NE1 | 2.49 | 0.46 |
| 1:BH:155:ARG:HG2 | 1:BH:156:ASP:O | 2.14 | 0.46 |
| 1:BH:235:GLU:C | 1:BH:236:PHE:HD1 | 2.19 | 0.46 |
| 1:BH:525:ASN:HB3 | 1:BH:528:THR:HG21 | 1.96 | 0.46 |
| 1:BI:349:VAL:HG13 | 1:BI:392:ILE:HD11 | 1.98 | 0.46 |
| 1:BI:563:VAL:HG12 | 1:BI:564:THR:O | 2.15 | 0.46 |
| 2:BJ:604:VAL:HG22 | 2:BJ:605:ARG:H | 1.80 | 0.46 |
| 2:C:193:MET:HB3 | 2:C:200:TYR:HB2 | 1.98 | 0.46 |
| 2:C:525:TRP:NE1 | 2:C:526:ILE:O | 2.49 | 0.46 |
| 2:C:555:ARG:HD2 | 2:C:557:VAL:O | 2.14 | 0.46 |
| 2:C:808:GLN:HE21 | 2:C:839:ILE:HG13 | 1.80 | 0.46 |
| 2:C:934:ALA:H | 2:C:997:SER:HB2 | 1.79 | 0.46 |
| 3:CB:76:MET:O | 3:CB:299:PRO:HD3 | 2.16 | 0.46 |
| 4:CC:67:TYR:CD1 | 4:CC:84:ARG:HB3 | 2.50 | 0.46 |
| 4:CD:39:TYR:CG | 4:CE:7:LYS:HD3 | 2.50 | 0.46 |
| 5:CG:313:PHE:CE2 | 5:CG:320:LEU:HD21 | 2.50 | 0.46 |
| 5:CH:151:ILE:HG23 | 5:CH:152:ASP:H | 1.81 | 0.46 |
| 5:CH:344:VAL:HG12 | 5:CH:349:TRP:H | 1.80 | 0.46 |
| 5:CH:344:VAL:O | 5:CH:345:LEU:HD12 | 2.16 | 0.46 |
| 6:CI:218:THR:HB | 7:FF:205:ARG:NH1 | 2.30 | 0.46 |
| 7:DB:32:VAL:HA | 7:DB:35:ALA:HB3 | 1.97 | 0.46 |
| 7:DB:71:ASN:O | 7:DB:73:THR:HG22 | 2.16 | 0.46 |
| 7:DD:7:GLN:HB3 | 7:DD:15:TYR:CE2 | 2.51 | 0.46 |
| 7:DB:346:ILE:HD11 | 7:DD:350:ALA:HB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:DF:112:ILE:HD11 | 8:DF:126:GLU:OE2 | 2.15 | 0.46 |
| 8:DF:114:ARG:HD2 | 8:DF:123:VAL:HG11 | 1.98 | 0.46 |
| 8:DF:122:THR:HG22 | 8:DF:123:VAL:H | 1.81 | 0.46 |
| 10:DH:203:ARG:NH2 | 10:DH:356:ARG:HH12 | 2.13 | 0.46 |
| 11:DI:190:LYS:O | 11:DI:193:GLY:N | 2.48 | 0.46 |
| 1:EA:5:PRO:HG3 | 1:EA:36:TRP:CZ2 | 2.49 | 0.46 |
| 1:EB:563:VAL:HG12 | 1:EB:564:THR:O | 2.15 | 0.46 |
| 2:EC:328:TYR:H | 2:EC:353:ASP:CG | 2.19 | 0.46 |
| 3:ED:153:CYS:O | 3:ED:158:GLY:N | 2.42 | 0.46 |
| 4:EF:107:VAL:O | 4:EF:148:LEU:N | 2.39 | 0.46 |
| 4:EG:8:LYS:HD2 | 4:EG:30:LYS:HA | 1.98 | 0.46 |
| 5:EJ:130:PHE:HB2 | 5:EJ:150:GLN:HB3 | 1.98 | 0.46 |
| 5:EJ:170:GLU:O | 5:EJ:172:GLN:N | 2.48 | 0.46 |
| 5:EJ:260:ARG:HA | 5:EJ:384:THR:HA | 1.98 | 0.46 |
| 5:EJ:507:ASP:OD2 | 5:EJ:511:ASN:HB2 | 2.14 | 0.46 |
| 4:F:139:VAL:HG13 | 4:F:164:ILE:HD12 | 1.97 | 0.46 |
| 5:FA:275:SER:OG | 5:FA:282:VAL:HG12 | 2.16 | 0.46 |
| 5:FA:289:LYS:HG3 | 5:FA:370:HIS:CE1 | 2.50 | 0.46 |
| 6:FC:70:ILE:HD11 | 6:FD:74:LYS:HG3 | 1.96 | 0.46 |
| 7:FE:266:THR:HG23 | 7:FE:281:LEU:HD23 | 1.97 | 0.46 |
| 7:FE:349:TRP:NE1 | 7:FE:351:ALA:HB3 | 2.30 | 0.46 |
| 7:FE:371:ASP:OD1 | 7:FE:526:LYS:NZ | 2.47 | 0.46 |
| 7:FE:493:GLU:HG3 | 7:FE:496:ARG:HH21 | 1.80 | 0.46 |
| 7:FG:375:TYR:CZ | 7:FG:392:LEU:HD23 | 2.50 | 0.46 |
| 7:FG:415:ASN:O | 7:FG:424:ARG:HD2 | 2.16 | 0.46 |
| 8:FH:70:THR:HG22 | 8:FH:156:THR:HG22 | 1.97 | 0.46 |
| 8:FH:40:ALA:O | 8:FH:69:TRP:NE1 | 2.49 | 0.46 |
| 4:G:139:VAL:HG13 | 4:G:164:ILE:HD12 | 1.97 | 0.46 |
| 1:GD:518:ASN:HA | 1:GD:535:LEU:HB3 | 1.96 | 0.46 |
| 1:GD:595:ILE:HG22 | 1:GD:602:ILE:HA | 1.98 | 0.46 |
| 1:GE:563:VAL:HG12 | 1:GE:564:THR:O | 2.15 | 0.46 |
| 2:GF:573:VAL:O | 2:GF:609:GLU:HA | 2.16 | 0.46 |
| 2:GF:934:ALA:H | 2:GF:997:SER:HB2 | 1.80 | 0.46 |
| 3:GG:197:ASP:OD1 | 3:GG:198:VAL:N | 2.45 | 0.46 |
| 4:GI:79:VAL:N | 4:GI:97:ILE:O | 2.32 | 0.46 |
| 4:H:8:LYS:HD2 | 4:H:30:LYS:HA | 1.98 | 0.46 |
| 4:GI:15:ILE:HD13 | 4:HA:25:PHE:HB2 | 1.97 | 0.46 |
| 5:HB:359:GLU:O | 5:HB:369:LEU:HA | 2.14 | 0.46 |
| 5:HB:518:GLY:N | 5:HD:594:THR:OG1 | 2.48 | 0.46 |
| 5:HC:460:TYR:CE2 | 5:HC:462:ASN:HB2 | 2.50 | 0.46 |
| 5:HD:110:VAL:HG22 | 5:HD:123:PRO:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:344:VAL:O | 5:HD:345:LEU:HD12 | 2.16 | 0.46 |
| 6:HF:7:LYS:HD3 | 6:HG:11:ILE:HA | 1.97 | 0.46 |
| 6:HF:10:VAL:HG22 | 6:HG:13:ARG:HB2 | 1.97 | 0.46 |
| 7:HH:195:THR:O | 7:HH:198:GLN:N | 2.48 | 0.46 |
| 7:HH:43:GLY:HA3 | 7:HI:39:ILE:HG23 | 1.97 | 0.46 |
| 7:HJ:157:THR:OG1 | 7:HJ:158:THR:N | 2.49 | 0.46 |
| 7:HJ:167:GLN:HG3 | 7:HJ:168:LEU:HG | 1.98 | 0.46 |
| 5:I:23:GLY:O | 5:I:24:ILE:HB | 2.15 | 0.46 |
| 5:I:318:GLN:NE2 | 6:N:4:LEU:HA | 2.30 | 0.46 |
| 8:IA:46:VAL:HG13 | 8:IA:63:ASP:O | 2.16 | 0.46 |
| 8:IB:40:ALA:O | 8:IB:69:TRP:NE1 | 2.49 | 0.46 |
| 10:ID:334:ILE:HG13 | 10:ID:335:ALA:N | 2.30 | 0.46 |
| 11:IE:111:TYR:HB3 | 11:IE:121:TYR:HD1 | 1.80 | 0.46 |
| 11:IE:190:LYS:O | 11:IE:193:GLY:N | 2.48 | 0.46 |
| 12:IF:223:VAL:HB | 12:IF:241:VAL:HG23 | 1.97 | 0.46 |
| 5:J:161:ASN:OD1 | 5:J:249:ASP:HB3 | 2.16 | 0.46 |
| 5:J:36:GLU:HA | 5:J:50:LYS:HZ1 | 1.79 | 0.46 |
| 5:K:164:ARG:HA | 5:K:181:PHE:CZ | 2.49 | 0.46 |
| 5:K:202:TYR:CZ | 5:K:225:LEU:HB2 | 2.49 | 0.46 |
| 5:K:264:ARG:HH22 | 6:L:2:SER:N | 2.14 | 0.46 |
| 7:O:323:GLY:HA2 | 7:P:326:ILE:HG23 | 1.96 | 0.46 |
| 7:O:329:ASN:HD21 | 7:Q:335:ASN:H | 1.63 | 0.46 |
| 1:X:235:GLU:C | 1:X:236:PHE:HD1 | 2.19 | 0.46 |
| 1:Y:118:LEU:HG | 1:Y:294:ASN:CG | 2.35 | 0.46 |
| 1:Y:455:PHE:CD2 | 1:Y:456:ASN:N | 2.83 | 0.46 |
| 13:YA:121[F]:TYR:HB3 | 13:YC:66[F]:MET:SD | 2.55 | 0.46 |
| 13:YA:148[A]:GLN:NE2 | 13:YA:421[A]:TYR:OH | 2.48 | 0.46 |
| 13:YA:370[A]:ASN:ND2 | 13:YA:372[A]:SER:HB3 | 2.29 | 0.46 |
| 13:YA:568[B]:ASP:OD1 | 13:YA:569[B]:GLY:N | 2.49 | 0.46 |
| 13:YA:81[D]:ARG:HB3 | 13:YA:100[D]:TYR:CZ | 2.50 | 0.46 |
| 13:YB:148[D]:GLN:NE2 | 13:YB:421[D]:TYR:OH | 2.48 | 0.46 |
| 13:YB:189[D]:LYS:HA | 13:YB:234[D]:GLY:O | 2.14 | 0.46 |
| 13:YA:70[F]:GLY:O | 13:YB:394[F]:GLU:N | 2.48 | 0.46 |
| 13:YB:567[E]:ILE:HG23 | 13:YC:565[E]:TYR:CD2 | 2.51 | 0.46 |
| 13:YB:568[F]:ASP:OD1 | 13:YB:569[F]:GLY:N | 2.49 | 0.46 |
| 13:YB:7[D]:ASN:OD1 | 13:YC:9[D]:ASN:ND2 | 2.49 | 0.46 |
| 13:YC:81[C]:ARG:HB3 | 13:YC:100[C]:TYR:CZ | 2.50 | 0.46 |
| 13:YC:148[B]:GLN:NE2 | 13:YC:421[B]:TYR:OH | 2.48 | 0.46 |
| 13:YC:148[D]:GLN:NE2 | 13:YC:421[D]:TYR:OH | 2.48 | 0.46 |
| 13:YC:24[D]:LEU:HD23 | 14:YF:259[D]:LEU:CD2 | 2.44 | 0.46 |
| 13:YB:69[A]:ILE:CD1 | 13:YC:396[A]:GLU:HA | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:69[E]:ILE:CD1 | 13:YC:396[E]:GLU:HA | 2.46 | 0.46 |
| 13:YA:464[D]:TYR:OH | 13:YC:454[D]:LYS:NZ | 2.48 | 0.46 |
| 13:YB:492[E]:GLY:HA3 | 13:YC:485[E]:ASP:HA | 1.98 | 0.46 |
| 13:YC:57[F]:VAL:HG21 | 13:YC:75[F]:GLY:HA3 | 1.98 | 0.46 |
| 13:YB:7[A]:ASN:OD1 | 13:YC:9[A]:ASN:ND2 | 2.48 | 0.46 |
| 14:YD:140[F]:TYR:CD2 | 14:YD:147[F]:THR:HA | 2.50 | 0.46 |
| 14:YD:160[B]:ILE:HG21 | 14:YD:282[B]:ALA:HB1 | 1.97 | 0.46 |
| 14:YD:214[A]:GLY:O | 14:YD:215[A]:GLU:HG3 | 2.15 | 0.46 |
| 14:YD:336[C]:GLU:O | 14:YD:359[C]:THR:OG1 | 2.33 | 0.46 |
| 14:YD:14[E]:VAL:HG11 | 14:YD:52[E]:LEU:HD11 | 1.97 | 0.46 |
| 14:YD:70[E]:ILE:N | 14:YD:88[E]:TYR:O | 2.49 | 0.46 |
| 11:V:175:SER:HA | 14:YE:217[E]:SER:HB2 | 1.98 | 0.46 |
| 11:DI:182:ASN:ND2 | 14:YE:327[B]:ASN:HD22 | 2.13 | 0.46 |
| 14:YE:10[E]:PRO:HD2 | 14:YE:349[E]:ASN:O | 2.15 | 0.46 |
| 14:YD:332[A]:GLN:HB3 | 14:YE:61[A]:HIS:NE2 | 2.30 | 0.46 |
| 14:YD:236[E]:TRP:N | 14:YE:95[E]:VAL:O | 2.49 | 0.46 |
| 14:YD:234[D]:PHE:HD1 | 14:YE:97[D]:VAL:HG12 | 1.80 | 0.46 |
| 14:YF:10[F]:PRO:HD2 | 14:YF:349[F]:ASN:O | 2.16 | 0.46 |
| 14:YF:117[B]:ASN:O | 14:YF:119[B]:LYS:HG3 | 2.16 | 0.46 |
| 14:YF:170[E]:LEU:HA | 14:YF:170[E]:LEU:HD23 | 1.68 | 0.46 |
| 14:YF:14[C]:VAL:HG11 | 14:YF:52[C]:LEU:HD11 | 1.97 | 0.46 |
| 14:YF:70[F]:ILE:N | 14:YF:88[F]:TYR:O | 2.49 | 0.46 |
| 2:Z:16:LEU:HD23 | 2:Z:102:THR:HA | 1.97 | 0.46 |
| 2:Z:562:ASP:O | 2:Z:565:ASP:N | 2.44 | 0.46 |
| 2:Z:569:VAL:HB | 2:Z:617:VAL:HG12 | 1.98 | 0.46 |
| 2:Z:664:PHE:O | 2:Z:667:PHE:HB3 | 2.15 | 0.46 |
| 15:ZA:2[D]:SER:HB3 | 15:ZA:77[D]:MET:HB3 | 1.96 | 0.46 |
| 1:A:155:ARG:HG2 | 1:A:156:ASP:O | 2.14 | 0.46 |
| 1:A:430:GLN:N | 1:A:430:GLN:OE1 | 2.29 | 0.46 |
| 1:A:654:ASP:OD1 | 1:A:655:LEU:N | 2.49 | 0.46 |
| 4:AA:67:TYR:CD1 | 4:AA:84:ARG:HB3 | 2.50 | 0.46 |
| 5:AC:313:PHE:HE2 | 5:AC:320:LEU:HD11 | 1.81 | 0.46 |
| 5:AC:402:GLU:HG3 | 5:AC:406:LEU:HD11 | 1.96 | 0.46 |
| 5:AC:87:ASN:HA | 5:AC:89:TYR:CE2 | 2.50 | 0.46 |
| 5:AD:116:THR:HA | 5:AD:121:ALA:HB2 | 1.96 | 0.46 |
| 5:AD:200:LEU:HD11 | 5:AE:241:THR:HG21 | 1.97 | 0.46 |
| 5:AD:358:VAL:HG23 | 5:AD:371:PHE:HD1 | 1.80 | 0.46 |
| 5:AC:486:VAL:HG12 | 5:AD:488:VAL:HG22 | 1.96 | 0.46 |
| 5:AE:96:ARG:NH1 | 5:AE:132:ASP:OD2 | 2.48 | 0.46 |
| 6:AG:32:ARG:NH1 | 6:AH:144:ASN:OD1 | 2.40 | 0.46 |
| 7:AI:342:PRO:HG2 | 7:AI:345:ALA:HB2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:323:GLY:HA2 | 7:AJ:326:ILE:HG23 | 1.96 | 0.46 |
| 7:AJ:50:ALA:HB3 | 7:AJ:58:LEU:HD12 | 1.97 | 0.46 |
| 1:B:209:TRP:CE3 | 1:B:212:LYS:HE3 | 2.51 | 0.46 |
| 7:AI:76:VAL:N | 7:BA:76:VAL:O | 2.34 | 0.46 |
| 8:BB:122:THR:HG22 | 8:BB:123:VAL:H | 1.81 | 0.46 |
| 8:BB:31:ASN:OD1 | 8:BB:32:PHE:N | 2.48 | 0.46 |
| 8:BB:40:ALA:O | 8:BB:69:TRP:NE1 | 2.49 | 0.46 |
| 11:BF:60:ALA:HB1 | 11:BF:69:LEU:O | 2.16 | 0.46 |
| 11:BF:56:PRO:HG3 | 11:BF:86:TRP:NE1 | 2.31 | 0.46 |
| 12:BG:214:VAL:HG23 | 12:BG:249:GLN:O | 2.15 | 0.46 |
| 1:BH:69:GLN:CD | 1:BI:21:PHE:HZ | 2.19 | 0.46 |
| 1:BI:386:THR:HG23 | 1:BI:387:VAL:N | 2.31 | 0.46 |
| 1:BI:572:TYR:HB2 | 1:BI:591:VAL:HG23 | 1.97 | 0.46 |
| 2:BJ:1002:ALA:HA | 5:CG:20:ARG:HB2 | 1.97 | 0.46 |
| 2:BJ:16:LEU:HD23 | 2:BJ:102:THR:HA | 1.96 | 0.46 |
| 2:BJ:389:ASN:O | 2:BJ:393:SER:OG | 2.21 | 0.46 |
| 2:BJ:664:PHE:O | 2:BJ:667:PHE:HB3 | 2.15 | 0.46 |
| 2:C:16:LEU:HD23 | 2:C:102:THR:HA | 1.97 | 0.46 |
| 2:C:968:ASP:HB3 | 2:C:972:GLU:CG | 2.42 | 0.46 |
| 3:CA:38:PHE:CD1 | 3:CA:80:LYS:HA | 2.49 | 0.46 |
| 4:CC:114:GLY:HA3 | 4:CC:143:TYR:CE2 | 2.49 | 0.46 |
| 4:CD:8:LYS:HD2 | 4:CD:30:LYS:HA | 1.98 | 0.46 |
| 4:CE:85:HIS:HD2 | 4:CE:109:PHE:HE1 | 1.62 | 0.46 |
| 5:CF:65:GLY:O | 5:CG:45:SER:OG | 2.26 | 0.46 |
| 2:BJ:984:SER:OG | 5:CG:12:ASP:OD2 | 2.13 | 0.46 |
| 5:CH:362:GLU:HG2 | 5:CH:368:ILE:HG22 | 1.96 | 0.46 |
| 5:CH:358:VAL:HG22 | 5:CH:371:PHE:HB2 | 1.98 | 0.46 |
| 5:CH:372:ASP:N | 5:CH:372:ASP:OD1 | 2.48 | 0.46 |
| 5:CH:71:ASN:OD1 | 5:CH:73:SER:N | 2.32 | 0.46 |
| 7:DB:475:LEU:HA | 7:DC:470:GLY:O | 2.16 | 0.46 |
| 7:DD:383:TYR:CE1 | 7:DD:393:PRO:HG3 | 2.50 | 0.46 |
| 8:DE:122:THR:HG22 | 8:DE:123:VAL:H | 1.81 | 0.46 |
| 10:DH:323:LYS:O | 10:DH:324:THR:OG1 | 2.33 | 0.46 |
| 10:DH:330:ASN:O | 10:DH:339:PRO:HA | 2.16 | 0.46 |
| 1:EA:182:LEU:O | 1:EA:182:LEU:HD12 | 2.15 | 0.46 |
| 1:EA:525:ASN:HB3 | 1:EA:528:THR:HG21 | 1.96 | 0.46 |
| 1:EB:256:TYR:N | 1:EB:256:TYR:CD1 | 2.83 | 0.46 |
| 1:EB:485:VAL:HG11 | 1:EB:650:TYR:HE1 | 1.79 | 0.46 |
| 2:EC:675:LEU:HD12 | 2:EC:675:LEU:HA | 1.67 | 0.46 |
| 2:EC:934:ALA:H | 2:EC:997:SER:HB2 | 1.80 | 0.46 |
| 4:EF:212:ARG:HG3 | 4:EF:213:LYS:HG3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:186:TYR:OH | 5:EI:190:ASN:O | 2.19 | 0.46 |
| 5:EI:186:TYR:HE1 | 5:EI:246:THR:HA | 1.80 | 0.46 |
| 5:EI:339:GLU:HG3 | 5:EI:340:VAL:HG13 | 1.96 | 0.46 |
| 5:EI:558:ASP:N | 5:EI:559:PRO:HD3 | 2.31 | 0.46 |
| 5:EI:87:ASN:HA | 5:EI:89:TYR:CE2 | 2.50 | 0.46 |
| 5:EJ:477:SER:HB2 | 5:EJ:602:ALA:HB3 | 1.96 | 0.46 |
| 5:FA:186:TYR:HD2 | 5:FA:227:GLY:HA2 | 1.80 | 0.46 |
| 6:FB:19:GLY:N | 6:FC:13:ARG:NH1 | 2.63 | 0.46 |
| 6:FC:76:GLY:HA2 | 6:FC:215:PHE:HZ | 1.79 | 0.46 |
| 6:FC:69:THR:HA | 6:FD:73:ASN:CB | 2.45 | 0.46 |
| 8:FI:122:THR:HG22 | 8:FI:123:VAL:H | 1.81 | 0.46 |
| 11:GB:178:ASN:H | 14:YD:217[E]:SER:C | 2.18 | 0.46 |
| 1:GD:174:ARG:HH21 | 1:GD:269:VAL:HG21 | 1.80 | 0.46 |
| 1:GE:386:THR:HG23 | 1:GE:387:VAL:N | 2.31 | 0.46 |
| 2:GF:10:SER:O | 2:GF:25:TRP:HA | 2.16 | 0.46 |
| 2:GF:146:LEU:HD11 | 2:GF:578:PHE:CE1 | 2.51 | 0.46 |
| 2:GF:654:PRO:HG3 | 9:IC:47:ARG:CD | 2.45 | 0.46 |
| 3:GG:153:CYS:O | 3:GG:158:GLY:N | 2.42 | 0.46 |
| 3:GH:71:MET:HG3 | 3:GH:271:GLN:NE2 | 2.29 | 0.46 |
| 3:GH:29:GLY:HA2 | 3:GH:34:LYS:HE3 | 1.97 | 0.46 |
| 3:GH:64:SER:HG | 3:GH:67:GLY:H | 1.57 | 0.46 |
| 4:GI:67:TYR:CD1 | 4:GI:84:ARG:HB3 | 2.50 | 0.46 |
| 5:HB:170:GLU:O | 5:HB:172:GLN:N | 2.48 | 0.46 |
| 5:HB:496:ASP:OD2 | 5:HB:499:PHE:HB2 | 2.15 | 0.46 |
| 5:HC:313:PHE:HB3 | 5:HC:381:ILE:HG12 | 1.98 | 0.46 |
| 5:HC:58:GLN:OE1 | 5:HC:58:GLN:N | 2.42 | 0.46 |
| 5:HD:104:VAL:HG13 | 5:HD:105:ASN:H | 1.80 | 0.46 |
| 5:HB:315:GLY:HA2 | 5:HD:317:LEU:O | 2.15 | 0.46 |
| 5:HD:335:ASP:N | 5:HD:335:ASP:OD1 | 2.47 | 0.46 |
| 5:HD:344:VAL:HG12 | 5:HD:349:TRP:H | 1.80 | 0.46 |
| 7:HH:302:ILE:HD12 | 7:HI:306:PHE:CZ | 2.50 | 0.46 |
| 7:HH:342:PRO:HG2 | 7:HH:345:ALA:HB2 | 1.96 | 0.46 |
| 7:HH:418:ASP:OD2 | 7:HI:505:PRO:HD3 | 2.15 | 0.46 |
| 7:HI:45:ASN:CG | 7:HJ:24:ASN:HD21 | 2.19 | 0.46 |
| 8:IA:69:TRP:CZ3 | 8:IA:157:LEU:HD12 | 2.51 | 0.46 |
| 5:J:146:VAL:HG11 | 5:K:151:ILE:O | 2.16 | 0.46 |
| 5:I:317:LEU:HD13 | 5:J:312:ARG:HH22 | 1.80 | 0.46 |
| 5:J:19:LEU:HD13 | 5:K:19:LEU:HD21 | 1.97 | 0.46 |
| 5:K:344:VAL:O | 5:K:345:LEU:HD12 | 2.16 | 0.46 |
| 6:M:203:LEU:HD12 | 6:M:206:GLN:NE2 | 2.31 | 0.46 |
| 6:N:168:LEU:HB2 | 6:N:180:GLN:OE1 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:138:SER:C | 7:Q:143:LYS:HG2 | 2.36 | 0.46 |
| 7:P:411:ASN:O | 7:P:415:ASN:ND2 | 2.48 | 0.46 |
| 7:Q:127:ASN:O | 7:Q:131:THR:HG23 | 2.15 | 0.46 |
| 7:P:45:ASN:CG | 7:Q:24:ASN:HD21 | 2.19 | 0.46 |
| 7:O:346:ILE:N | 7:Q:348:MET:O | 2.29 | 0.46 |
| 7:Q:87:TYR:CZ | 7:Q:97:LEU:HD12 | 2.51 | 0.46 |
| 1:X:231:ASP:OD1 | 1:X:233:ASN:N | 2.36 | 0.46 |
| 1:X:68:GLN:HA | 2:Z:682:GLN:NE2 | 2.30 | 0.46 |
| 13:YA:121[E]:TYR:HB3 | 13:YC:66[E]:MET:SD | 2.56 | 0.46 |
| 13:YA:266[B]:TRP:CD1 | 13:YA:274[B]:GLN:HG2 | 2.51 | 0.46 |
| 13:YA:304[B]:TRP:O | 13:YA:308[B]:TYR:N | 2.33 | 0.46 |
| 13:YA:337[E]:GLU:O | 13:YA:340[E]:GLY:N | 2.48 | 0.46 |
| 13:YA:550[B]:TRP:O | 13:YC:558[B]:SER:N | 2.48 | 0.46 |
| 13:YA:550[F]:TRP:O | 13:YC:558[F]:SER:N | 2.48 | 0.46 |
| 13:YA:558[B]:SER:O | 13:YB:551[B]:THR:HA | 2.16 | 0.46 |
| 13:YA:568[E]:ASP:OD1 | 13:YA:569[E]:GLY:N | 2.49 | 0.46 |
| 13:YA:568[C]:ASP:OD1 | 13:YA:569[C]:GLY:N | 2.49 | 0.46 |
| 13:YB:109[B]:ASN:OD1 | 13:YB:111[B]:LEU:N | 2.49 | 0.46 |
| 13:YB:146[A]:VAL:O | 13:YB:150[A]:SER:OG | 2.34 | 0.46 |
| 13:YB:266[E]:TRP:CD1 | 13:YB:274[E]:GLN:HG2 | 2.51 | 0.46 |
| 13:YB:44[F]:VAL:HG11 | 14:YD:272[F]:GLU:HB3 | 1.96 | 0.46 |
| 13:YB:561[A]:SER:HA | 13:YC:554[A]:MET:O | 2.16 | 0.46 |
| 13:YB:567[B]:ILE:HG23 | 13:YC:565[B]:TYR:CD2 | 2.50 | 0.46 |
| 13:YB:568[C]:ASP:OD1 | 13:YB:569[C]:GLY:N | 2.49 | 0.46 |
| 13:YB:66[F]:MET:HE2 | 13:YC:122[F]:PRO:HB3 | 1.97 | 0.46 |
| 13:YB:57[F]:VAL:HG21 | 13:YB:75[F]:GLY:HA3 | 1.98 | 0.46 |
| 13:YA:61[E]:ILE:HG22 | 13:YB:76[E]:PRO:C | 2.35 | 0.46 |
| 13:YC:266[E]:TRP:CD1 | 13:YC:274[E]:GLN:HG2 | 2.51 | 0.46 |
| 13:YB:315[C]:LEU:HD23 | 13:YC:367[C]:PRO:HA | 1.97 | 0.46 |
| 13:YB:69[E]:ILE:HG12 | 13:YC:396[E]:GLU:HA | 1.97 | 0.46 |
| 13:YC:39[B]:ARG:NH1 | 13:YC:113[B]:GLY:HA2 | 2.30 | 0.46 |
| 13:YC:39[E]:ARG:NH1 | 13:YC:113[E]:GLY:HA2 | 2.30 | 0.46 |
| 13:YC:148[A]:GLN:NE2 | 13:YC:421[A]:TYR:OH | 2.48 | 0.46 |
| 13:YB:481[C]:PHE:O | 13:YC:473[C]:GLN:HA | 2.15 | 0.46 |
| 13:YB:551[A]:THR:O | 13:YC:543[A]:ASP:HA | 2.16 | 0.46 |
| 13:YA:393[D]:MET:HA | 13:YC:71[D]:GLY:HA2 | 1.98 | 0.46 |
| 13:YC:81[F]:ARG:HB3 | 13:YC:100[F]:TYR:CZ | 2.50 | 0.46 |
| 14:YD:117[A]:ASN:O | 14:YD:119[A]:LYS:HG3 | 2.16 | 0.46 |
| 14:YD:14[C]:VAL:HG11 | 14:YD:52[C]:LEU:HD11 | 1.97 | 0.46 |
| 14:YD:14[F]:VAL:HG11 | 14:YD:52[F]:LEU:HD11 | 1.96 | 0.46 |
| 14:YD:15[A]:LYS:HE2 | 14:YD:15[A]:LYS:HB3 | 1.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:IE:182:ASN:ND2 | 14:YD:327[F]:ASN:HD22 | 2.13 | 0.46 |
| 14:YD:20[B]:TYR:HA | 14:YD:69[B]:ILE:HD12 | 1.98 | 0.46 |
| 14:YD:95[A]:VAL:O | 14:YF:236[A]:TRP:N | 2.49 | 0.46 |
| 14:YE:140[C]:TYR:CD2 | 14:YE:147[C]:THR:HA | 2.50 | 0.46 |
| 10:BE:285:LEU:HA | 14:YE:215[A]:GLU:HG3 | 1.94 | 0.46 |
| 14:YE:31[A]:LEU:O | 14:YE:35[A]:ILE:HG22 | 2.14 | 0.46 |
| 14:YE:20[B]:TYR:HA | 14:YE:69[B]:ILE:HD12 | 1.98 | 0.46 |
| 14:YF:117[A]:ASN:O | 14:YF:119[A]:LYS:HG3 | 2.16 | 0.46 |
| 14:YF:140[B]:TYR:CD2 | 14:YF:147[B]:THR:HA | 2.50 | 0.46 |
| 14:YF:14[E]:VAL:HG11 | 14:YF:52[E]:LEU:HD11 | 1.96 | 0.46 |
| 13:YC:24[F]:LEU:HD23 | 14:YF:259[F]:LEU:CD2 | 2.45 | 0.46 |
| 14:YF:160[B]:ILE:HG21 | 14:YF:282[B]:ALA:HB1 | 1.97 | 0.46 |
| 14:YF:212[D]:ILE:HG22 | 14:YF:327[D]:ASN:HB2 | 1.96 | 0.46 |
| 14:YF:31[E]:LEU:O | 14:YF:35[E]:ILE:HG22 | 2.14 | 0.46 |
| 14:YF:70[A]:ILE:N | 14:YF:88[A]:TYR:O | 2.49 | 0.46 |
| 2:Z:151:PHE:CD2 | 2:Z:166:PHE:HE1 | 2.33 | 0.46 |
| 2:Z:555:ARG:HD2 | 2:Z:557:VAL:O | 2.14 | 0.46 |
| 2:Z:808:GLN:HE21 | 2:Z:839:ILE:HG13 | 1.80 | 0.46 |
| 1:A:10:LEU:O | 1:A:11:THR:OG1 | 2.31 | 0.46 |
| 1:A:571:PRO:HA | 1:A:589:TYR:O | 2.15 | 0.46 |
| 1:A:595:ILE:HG22 | 1:A:602:ILE:HA | 1.98 | 0.46 |
| 5:AC:19:LEU:HD12 | 5:AC:20:ARG:N | 2.31 | 0.46 |
| 5:AC:289:LYS:HD2 | 5:AC:372:ASP:HB3 | 1.98 | 0.46 |
| 5:AD:356:TYR:HE1 | 6:AF:4:LEU:HD13 | 1.81 | 0.46 |
| 5:AD:97:ASP:OD1 | 5:AD:102:TRP:CE2 | 2.68 | 0.46 |
| 5:AE:151:ILE:HG23 | 5:AE:152:ASP:H | 1.81 | 0.46 |
| 5:AE:316:ILE:HD13 | 6:AG:7:LYS:HG3 | 1.98 | 0.46 |
| 5:AE:362:GLU:HG2 | 5:AE:368:ILE:HG22 | 1.96 | 0.46 |
| 6:AG:203:LEU:HD12 | 6:AG:206:GLN:NE2 | 2.31 | 0.46 |
| 7:AI:101:SER:HA | 7:AI:105:GLU:OE1 | 2.16 | 0.46 |
| 7:AI:147:LEU:HB2 | 7:AI:148:PRO:HD3 | 1.97 | 0.46 |
| 7:AJ:119:ALA:O | 7:AJ:122:THR:OG1 | 2.24 | 0.46 |
| 7:AJ:11:ASN:OD1 | 7:AJ:11:ASN:N | 2.48 | 0.46 |
| 7:AJ:348:MET:SD | 7:BA:400:VAL:HG11 | 2.56 | 0.46 |
| 7:AJ:31:ASP:CG | 7:AJ:34:ALA:H | 2.18 | 0.46 |
| 7:AJ:411:ASN:O | 7:AJ:415:ASN:ND2 | 2.48 | 0.46 |
| 1:B:49:GLU:HA | 1:B:54:ASN:ND2 | 2.28 | 0.46 |
| 1:B:563:VAL:HG12 | 1:B:564:THR:O | 2.15 | 0.46 |
| 8:BB:69:TRP:CZ3 | 8:BB:157:LEU:HD12 | 2.51 | 0.46 |
| 10:BE:330:ASN:O | 10:BE:339:PRO:HA | 2.16 | 0.46 |
| 12:BG:120:SER:HA | 12:BG:123:LEU:HG | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:174:ARG:HH21 | 1:BH:269:VAL:HG21 | 1.80 | 0.46 |
| 1:BI:175:THR:O | 1:BI:270:ILE:HG22 | 2.15 | 0.46 |
| 1:BI:209:TRP:CE3 | 1:BI:212:LYS:HE3 | 2.51 | 0.46 |
| 1:BI:23:GLY:O | 1:BI:29:ILE:HD11 | 2.16 | 0.46 |
| 2:BJ:328:TYR:H | 2:BJ:353:ASP:CG | 2.19 | 0.46 |
| 2:BJ:39:ALA:HB2 | 2:BJ:56:TRP:CE3 | 2.51 | 0.46 |
| 2:BJ:146:LEU:HD11 | 2:BJ:578:PHE:CE1 | 2.51 | 0.46 |
| 2:BJ:706:SER:O | 2:BJ:708:ILE:N | 2.42 | 0.46 |
| 2:BJ:78:TYR:HB2 | 2:BJ:100:PHE:CZ | 2.50 | 0.46 |
| 3:CA:257:TYR:HB3 | 3:CA:296:TYR:CE2 | 2.50 | 0.46 |
| 3:CA:71:MET:HE1 | 3:CA:271:GLN:HG2 | 1.97 | 0.46 |
| 3:CB:219:ASP:CG | 3:CB:222:ARG:H | 2.19 | 0.46 |
| 5:CF:289:LYS:HD2 | 5:CF:372:ASP:HB3 | 1.98 | 0.46 |
| 5:CF:399:ILE:HD12 | 5:CH:399:ILE:HG12 | 1.97 | 0.46 |
| 5:CF:49:TRP:HB2 | 5:CH:90:ASN:OD1 | 2.16 | 0.46 |
| 5:CG:107:VAL:O | 5:CG:125:GLU:HG3 | 2.16 | 0.46 |
| 5:CG:313:PHE:HB3 | 5:CG:381:ILE:HG12 | 1.98 | 0.46 |
| 5:CH:275:SER:OG | 5:CH:282:VAL:HG12 | 2.16 | 0.46 |
| 5:CF:98:VAL:HG11 | 5:CH:89:TYR:HB3 | 1.97 | 0.46 |
| 6:CI:29:VAL:O | 6:CI:32:ARG:N | 2.36 | 0.46 |
| 6:CI:32:ARG:NH1 | 6:CJ:144:ASN:OD1 | 2.42 | 0.46 |
| 3:D:246:THR:HA | 3:D:332:PHE:O | 2.15 | 0.46 |
| 3:D:42:GLY:HA2 | 3:D:76:MET:HG3 | 1.97 | 0.46 |
| 7:DB:12:GLU:HG3 | 7:DB:14:ARG:N | 2.31 | 0.46 |
| 7:DB:42:ALA:HB3 | 7:DD:43:GLY:O | 2.15 | 0.46 |
| 7:DC:228:ILE:HG21 | 7:DC:244:ALA:HB2 | 1.97 | 0.46 |
| 7:DB:357:ASP:OD1 | 7:DC:339:ARG:NH2 | 2.48 | 0.46 |
| 7:DC:478:ASP:CG | 7:DD:454:HIS:HE2 | 2.19 | 0.46 |
| 7:DB:447:HIS:CD2 | 7:DD:447:HIS:CD2 | 3.03 | 0.46 |
| 7:DB:462:ASN:HB3 | 7:DD:482:TYR:HD1 | 1.81 | 0.46 |
| 8:DE:79:HIS:HE1 | 8:DE:151:GLN:HE22 | 1.63 | 0.46 |
| 8:DF:79:HIS:CE1 | 8:DF:151:GLN:HE22 | 2.33 | 0.46 |
| 8:DF:46:VAL:HG13 | 8:DF:63:ASP:O | 2.15 | 0.46 |
| 11:DI:2:LEU:HD12 | 11:DI:2:LEU:N | 2.30 | 0.46 |
| 3:E:321:ALA:O | 3:E:324:GLN:HB3 | 2.15 | 0.46 |
| 1:EA:444:ILE:O | 1:EA:447:TYR:HB3 | 2.16 | 0.46 |
| 1:EA:518:ASN:OD1 | 1:EA:519:SER:N | 2.48 | 0.46 |
| 1:EA:571:PRO:HA | 1:EA:589:TYR:O | 2.15 | 0.46 |
| 1:EB:182:LEU:HD12 | 1:EB:182:LEU:O | 2.16 | 0.46 |
| 1:EB:386:THR:HG23 | 1:EB:387:VAL:N | 2.31 | 0.46 |
| 1:EB:356:ILE:HG21 | 1:EB:388:GLN:NE2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:EE:217:LYS:HA | 3:EE:236:PHE:CE2 | 2.51 | 0.46 |
| 4:EF:178:THR:HA | 4:EF:275:ALA:HA | 1.97 | 0.46 |
| 4:EG:212:ARG:HG3 | 4:EG:213:LYS:HG3 | 1.96 | 0.46 |
| 5:EI:196:ARG:O | 5:FA:197:GLY:HA2 | 2.16 | 0.46 |
| 5:EI:19:LEU:HD12 | 5:EI:20:ARG:N | 2.31 | 0.46 |
| 5:EJ:322:GLY:HA2 | 5:EJ:360:THR:H | 1.81 | 0.46 |
| 4:F:8:LYS:HD2 | 4:F:30:LYS:HA | 1.98 | 0.46 |
| 6:FB:203:LEU:HD12 | 6:FB:206:GLN:NE2 | 2.31 | 0.46 |
| 6:FC:44:ALA:HA | 6:FD:110:PHE:C | 2.35 | 0.46 |
| 7:FE:382:ARG:HH22 | 7:FE:434:VAL:HB | 1.81 | 0.46 |
| 7:FE:462:ASN:HB3 | 7:FG:482:TYR:HD1 | 1.81 | 0.46 |
| 7:FF:170:ILE:HG23 | 7:FG:173:ILE:HD13 | 1.97 | 0.46 |
| 7:FF:371:ASP:OD1 | 7:FF:526:LYS:NZ | 2.45 | 0.46 |
| 7:FG:157:THR:OG1 | 7:FG:158:THR:N | 2.49 | 0.46 |
| 7:FG:167:GLN:HG3 | 7:FG:168:LEU:HG | 1.98 | 0.46 |
| 8:FH:122:THR:HG22 | 8:FH:123:VAL:H | 1.81 | 0.46 |
| 8:FI:69:TRP:CZ3 | 8:FI:157:LEU:HD12 | 2.51 | 0.46 |
| 8:FI:70:THR:HG22 | 8:FI:156:THR:HG22 | 1.98 | 0.46 |
| 4:G:67:TYR:CD1 | 4:G:84:ARG:HB3 | 2.50 | 0.46 |
| 10:GA:287:VAL:O | 14:YD:100[A]:LYS:HD3 | 2.15 | 0.46 |
| 1:GE:491:PHE:CE2 | 1:GE:619:GLN:HA | 2.51 | 0.46 |
| 2:GF:319:TYR:HD1 | 2:GF:328:TYR:CB | 2.29 | 0.46 |
| 2:GF:339:ASP:O | 2:GF:341:LEU:N | 2.47 | 0.46 |
| 2:GF:231:TYR:CE1 | 2:GF:391:ARG:HD3 | 2.48 | 0.46 |
| 3:GG:177:GLU:HG3 | 3:GG:179:THR:H | 1.80 | 0.46 |
| 3:GG:92:ARG:NH1 | 3:GG:94:ASP:OD2 | 2.44 | 0.46 |
| 4:GI:178:THR:HA | 4:GI:275:ALA:HA | 1.97 | 0.46 |
| 5:HB:571:GLU:OE2 | 5:HD:567:THR:HG21 | 2.15 | 0.46 |
| 5:HC:265:LEU:HG | 5:HC:379:ASP:HB2 | 1.98 | 0.46 |
| 5:HC:322:GLY:HA2 | 5:HC:360:THR:H | 1.81 | 0.46 |
| 5:HC:36:GLU:HA | 5:HC:50:LYS:HZ1 | 1.79 | 0.46 |
| 5:HB:416:ILE:HG23 | 5:HD:472:TYR:HA | 1.97 | 0.46 |
| 6:HE:126:VAL:HG12 | 6:HE:130:ARG:NH1 | 2.31 | 0.46 |
| 6:HF:203:LEU:HD12 | 6:HF:206:GLN:NE2 | 2.31 | 0.46 |
| 6:HF:76:GLY:HA2 | 6:HF:215:PHE:HZ | 1.79 | 0.46 |
| 7:HH:32:VAL:HA | 7:HH:35:ALA:HB3 | 1.97 | 0.46 |
| 7:HH:77:THR:OG1 | 7:HH:78:PRO:HD2 | 2.16 | 0.46 |
| 7:HJ:375:TYR:CZ | 7:HJ:392:LEU:HD23 | 2.50 | 0.46 |
| 5:I:289:LYS:HD2 | 5:I:372:ASP:HB3 | 1.98 | 0.46 |
| 5:I:316:ILE:HG22 | 5:I:318:GLN:HG3 | 1.97 | 0.46 |
| 10:ID:323:LYS:O | 10:ID:324:THR:OG1 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:IF:196:GLU:OE2 | 12:IF:217:THR:HG23 | 2.15 | 0.46 |
| 5:J:107:VAL:O | 5:J:125:GLU:HG3 | 2.16 | 0.46 |
| 5:J:260:ARG:HA | 5:J:384:THR:HA | 1.98 | 0.46 |
| 5:J:313:PHE:HE2 | 5:J:320:LEU:HD11 | 1.80 | 0.46 |
| 5:J:358:VAL:HG23 | 5:J:371:PHE:HD1 | 1.80 | 0.46 |
| 6:L:10:VAL:HG11 | 6:N:10:VAL:HG21 | 1.98 | 0.46 |
| 7:O:130:GLU:OE2 | 7:P:132:ARG:NH1 | 2.39 | 0.46 |
| 7:O:32:VAL:O | 7:O:36:ILE:N | 2.39 | 0.46 |
| 7:O:71:ASN:O | 7:O:73:THR:HG22 | 2.16 | 0.46 |
| 7:Q:157:THR:OG1 | 7:Q:158:THR:N | 2.49 | 0.46 |
| 7:Q:325:TYR:CD1 | 7:Q:330:ARG:HA | 2.45 | 0.46 |
| 7:O:84:ARG:NH1 | 7:Q:85:LEU:HD22 | 2.30 | 0.46 |
| 11:V:56:PRO:HG3 | 11:V:86:TRP:NE1 | 2.31 | 0.46 |
| 1:X:571:PRO:HA | 1:X:589:TYR:O | 2.15 | 0.46 |
| 1:X:67:ILE:HD11 | 1:Y:67:ILE:HG21 | 1.98 | 0.46 |
| 13:YA:81[F]:ARG:HB3 | 13:YA:100[F]:TYR:CZ | 2.50 | 0.46 |
| 13:YA:121[B]:TYR:HB3 | 13:YC:66[B]:MET:SD | 2.55 | 0.46 |
| 13:YA:122[D]:PRO:HB3 | 13:YC:66[D]:MET:HE2 | 1.96 | 0.46 |
| 13:YA:189[F]:LYS:HA | 13:YA:234[F]:GLY:O | 2.14 | 0.46 |
| 13:YA:257[C]:LYS:HE2 | 13:YA:266[C]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YA:266[C]:TRP:CD1 | 13:YA:274[C]:GLN:HG2 | 2.51 | 0.46 |
| 13:YA:39[C]:ARG:NH1 | 13:YA:113[C]:GLY:HA2 | 2.30 | 0.46 |
| 13:YA:148[E]:GLN:NE2 | 13:YA:421[E]:TYR:OH | 2.48 | 0.46 |
| 13:YA:470[D]:ARG:HD2 | 13:YC:474[D]:ILE:HD11 | 1.97 | 0.46 |
| 13:YA:558[A]:SER:O | 13:YB:551[A]:THR:HA | 2.16 | 0.46 |
| 13:YA:61[C]:ILE:HG21 | 13:YB:59[C]:GLN:CA | 2.40 | 0.46 |
| 13:YA:66[D]:MET:HE2 | 13:YB:122[D]:PRO:HB3 | 1.97 | 0.46 |
| 13:YA:567[E]:ILE:HG23 | 13:YB:565[E]:TYR:CE2 | 2.50 | 0.46 |
| 13:YC:189[B]:LYS:HA | 13:YC:234[B]:GLY:O | 2.14 | 0.46 |
| 13:YC:337[A]:GLU:O | 13:YC:340[A]:GLY:N | 2.48 | 0.46 |
| 13:YA:447[C]:ASN:HB3 | 13:YC:376[C]:PHE:CZ | 2.50 | 0.46 |
| 13:YC:416[A]:HIS:CG | 13:YC:417[A]:PRO:HD2 | 2.51 | 0.46 |
| 13:YC:490[F]:VAL:HG12 | 13:YC:492[F]:GLY:H | 1.81 | 0.46 |
| 13:YB:561[B]:SER:HA | 13:YC:554[B]:MET:O | 2.16 | 0.46 |
| 13:YB:561[C]:SER:HA | 13:YC:554[C]:MET:O | 2.16 | 0.46 |
| 13:YC:568[E]:ASP:OD1 | 13:YC:569[E]:GLY:N | 2.49 | 0.46 |
| 13:YB:60[F]:PRO:HB3 | 13:YC:60[F]:PRO:HB3 | 1.96 | 0.46 |
| 13:YC:18[B]:ARG:CZ | 13:YC:77[B]:VAL:HG23 | 2.46 | 0.46 |
| 14:YD:101[F]:GLY:HA3 | 14:YF:330[F]:LYS:HG2 | 1.96 | 0.46 |
| 14:YD:109[C]:LEU:HD12 | 14:YD:109[C]:LEU:HA | 1.65 | 0.46 |
| 14:YD:178[E]:LEU:CD1 | 14:YD:183[E]:ASP:HA | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:V:175:SER:HA | 14:YD:217[A]:SER:HB2 | 1.98 | 0.46 |
| 14:YD:31[C]:LEU:O | 14:YD:35[C]:ILE:HG22 | 2.14 | 0.46 |
| 14:YD:70[B]:ILE:N | 14:YD:88[B]:TYR:O | 2.49 | 0.46 |
| 14:YD:70[A]:ILE:N | 14:YD:88[A]:TYR:O | 2.49 | 0.46 |
| 14:YE:140[E]:TYR:CD2 | 14:YE:147[E]:THR:HA | 2.50 | 0.46 |
| 14:YE:15[E]:LYS:HE2 | 14:YE:15[E]:LYS:HB3 | 1.54 | 0.46 |
| 14:YE:236[C]:TRP:CD1 | 14:YE:308[C]:ALA:HB2 | 2.51 | 0.46 |
| 14:YE:38[F]:LEU:HD12 | 14:YE:38[F]:LEU:HA | 1.63 | 0.46 |
| 14:YE:70[E]:ILE:N | 14:YE:88[E]:TYR:O | 2.49 | 0.46 |
| 14:YE:70[C]:ILE:N | 14:YE:88[C]:TYR:O | 2.49 | 0.46 |
| 14:YE:70[D]:ILE:N | 14:YE:88[D]:TYR:O | 2.49 | 0.46 |
| 14:YF:117[C]:ASN:O | 14:YF:119[C]:LYS:HG3 | 2.16 | 0.46 |
| 14:YF:20[F]:TYR:HA | 14:YF:69[F]:ILE:HD12 | 1.98 | 0.46 |
| 14:YF:212[F]:ILE:HG22 | 14:YF:327[F]:ASN:HB2 | 1.97 | 0.46 |
| 11:DI:178:ASN:HB3 | 14:YF:217[F]:SER:H | 1.81 | 0.46 |
| 14:YF:236[B]:TRP:CD1 | 14:YF:308[B]:ALA:HB2 | 2.51 | 0.46 |
| 14:YF:336[C]:GLU:O | 14:YF:359[C]:THR:OG1 | 2.33 | 0.46 |
| 14:YF:14[B]:VAL:HG11 | 14:YF:52[B]:LEU:HD11 | 1.96 | 0.46 |
| 14:YF:70[B]:ILE:N | 14:YF:88[B]:TYR:O | 2.49 | 0.46 |
| 14:YF:70[D]:ILE:N | 14:YF:88[D]:TYR:O | 2.49 | 0.46 |
| 2:Z:548:ILE:N | 2:Z:549:PRO:HD3 | 2.30 | 0.46 |
| 2:Z:573:VAL:O | 2:Z:609:GLU:HA | 2.16 | 0.46 |
| 2:Z:78:TYR:HB2 | 2:Z:100:PHE:CZ | 2.50 | 0.46 |
| 4:AA:64:THR:N | 4:AB:82:GLY:O | 2.37 | 0.46 |
| 5:AC:182:ARG:NH1 | 5:AD:299:ILE:HG12 | 2.29 | 0.46 |
| 5:AC:334:ALA:HA | 5:AC:349:TRP:NE1 | 2.31 | 0.46 |
| 5:AC:573:LYS:HD3 | 5:AD:537:THR:O | 2.16 | 0.46 |
| 5:AE:289:LYS:HG3 | 5:AE:370:HIS:CE1 | 2.50 | 0.46 |
| 5:AE:335:ASP:N | 5:AE:335:ASP:OD1 | 2.47 | 0.46 |
| 6:AF:168:LEU:HB2 | 6:AF:180:GLN:OE1 | 2.15 | 0.46 |
| 7:AI:468:PHE:HB2 | 7:BA:479:ASN:O | 2.15 | 0.46 |
| 7:AJ:118:PRO:HG3 | 7:BA:106:ALA:HA | 1.96 | 0.46 |
| 7:AJ:85:LEU:HD23 | 7:AJ:85:LEU:O | 2.15 | 0.46 |
| 8:BB:114:ARG:HD2 | 8:BB:123:VAL:HG11 | 1.97 | 0.46 |
| 8:BC:14:ASP:CG | 8:BC:17:ARG:HH22 | 2.18 | 0.46 |
| 10:BE:207:PHE:O | 10:BE:345:GLU:HA | 2.16 | 0.46 |
| 1:BH:167:LEU:HA | 1:BH:167:LEU:HD23 | 1.76 | 0.46 |
| 1:BH:252:LEU:HD12 | 1:BH:252:LEU:O | 2.15 | 0.46 |
| 2:BJ:151:PHE:CD2 | 2:BJ:166:PHE:HE1 | 2.33 | 0.46 |
| 2:BJ:825:GLU:HA | 2:BJ:836:GLY:O | 2.16 | 0.46 |
| 2:C:146:LEU:HD11 | 2:C:578:PHE:CE1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:120:ASN:CB | 2:C:155:PRO:HB3 | 2.35 | 0.46 |
| 2:C:569:VAL:HB | 2:C:617:VAL:HG12 | 1.98 | 0.46 |
| 5:CF:206:PHE:CD2 | 5:CF:223:VAL:HA | 2.50 | 0.46 |
| 5:CF:348:THR:H | 7:FE:233:GLN:HG3 | 1.81 | 0.46 |
| 5:CG:130:PHE:HB2 | 5:CG:150:GLN:HB3 | 1.98 | 0.46 |
| 5:CF:573:LYS:HD3 | 5:CG:537:THR:O | 2.16 | 0.46 |
| 5:CH:117:ILE:HG22 | 5:CH:143:TRP:HE3 | 1.80 | 0.46 |
| 5:CH:186:TYR:HD2 | 5:CH:227:GLY:HA2 | 1.80 | 0.46 |
| 6:CI:203:LEU:HD12 | 6:CI:206:GLN:NE2 | 2.31 | 0.46 |
| 6:DA:126:VAL:HG12 | 6:DA:130:ARG:NH1 | 2.31 | 0.46 |
| 7:DB:424:ARG:O | 7:DC:504:ARG:NH2 | 2.49 | 0.46 |
| 7:DB:190:VAL:HG23 | 7:DC:188:GLN:HB3 | 1.97 | 0.46 |
| 7:DC:50:ALA:HB3 | 7:DC:58:LEU:HD12 | 1.97 | 0.46 |
| 7:DC:66:VAL:HG11 | 7:DC:80:THR:HB | 1.98 | 0.46 |
| 7:DD:418:ASP:OD2 | 7:DD:422:LYS:HB2 | 2.16 | 0.46 |
| 8:DE:112:ILE:HD11 | 8:DE:126:GLU:OE2 | 2.15 | 0.46 |
| 8:DE:46:VAL:HG13 | 8:DE:63:ASP:O | 2.16 | 0.46 |
| 9:DG:58:SER:O | 9:DG:62:PHE:N | 2.34 | 0.46 |
| 1:EA:179:TYR:HD1 | 1:EA:185:ILE:HD11 | 1.80 | 0.46 |
| 1:EA:427:ASN:OD1 | 1:EA:428:LYS:N | 2.49 | 0.46 |
| 1:EA:565:GLU:HB3 | 1:EA:570:GLN:OE1 | 2.16 | 0.46 |
| 2:EC:10:SER:O | 2:EC:25:TRP:HA | 2.16 | 0.46 |
| 2:EC:180:ILE:HG23 | 2:EC:201:LEU:HD11 | 1.97 | 0.46 |
| 2:EC:784:GLN:HG2 | 2:EC:830:ARG:HG2 | 1.95 | 0.46 |
| 3:EE:95:TRP:CH2 | 3:EE:169:PRO:HD3 | 2.51 | 0.46 |
| 3:ED:310:ILE:HB | 3:EE:16:PHE:HB2 | 1.96 | 0.46 |
| 5:EI:315:GLY:HA2 | 5:FA:317:LEU:O | 2.16 | 0.46 |
| 5:EJ:107:VAL:O | 5:EJ:125:GLU:HG3 | 2.16 | 0.46 |
| 5:EJ:304:ILE:HD13 | 5:EJ:309:LEU:HG | 1.97 | 0.46 |
| 5:EJ:400:ILE:HG12 | 5:FA:402:GLU:OE2 | 2.15 | 0.46 |
| 4:F:85:HIS:HD2 | 4:F:109:PHE:HE1 | 1.62 | 0.46 |
| 5:FA:117:ILE:HG22 | 5:FA:143:TRP:CE3 | 2.50 | 0.46 |
| 5:EJ:395:THR:HG22 | 5:FA:307:ASN:HD21 | 1.81 | 0.46 |
| 7:FF:66:VAL:HG11 | 7:FF:80:THR:HB | 1.98 | 0.46 |
| 7:FG:221:THR:HG23 | 7:FG:223:GLU:H | 1.80 | 0.46 |
| 7:FE:321:MET:HA | 7:FG:315:ILE:O | 2.16 | 0.46 |
| 4:G:168:PHE:CE1 | 4:H:161:ASN:HB3 | 2.50 | 0.46 |
| 11:GB:111:TYR:HB3 | 11:GB:121:TYR:HD1 | 1.80 | 0.46 |
| 11:GB:2:LEU:HD12 | 11:GB:2:LEU:N | 2.30 | 0.46 |
| 1:GD:10:LEU:HD11 | 2:GF:701:TRP:HB3 | 1.97 | 0.46 |
| 1:GD:182:LEU:O | 1:GD:182:LEU:HD12 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:235:GLU:C | 1:GD:236:PHE:HD1 | 2.19 | 0.46 |
| 1:GD:554:ILE:HG22 | 1:GD:555:ILE:O | 2.16 | 0.46 |
| 1:GE:209:TRP:CE3 | 1:GE:212:LYS:HE3 | 2.51 | 0.46 |
| 1:GE:209:TRP:NE1 | 1:GE:223:ILE:HG12 | 2.30 | 0.46 |
| 1:GE:351:GLU:N | 1:GE:351:GLU:OE1 | 2.48 | 0.46 |
| 1:GE:356:ILE:HG21 | 1:GE:388:GLN:NE2 | 2.30 | 0.46 |
| 2:GF:254:PHE:HB3 | 2:GF:294:PHE:HB3 | 1.96 | 0.46 |
| 2:GF:479:TRP:CE2 | 2:GF:505:PRO:HA | 2.50 | 0.46 |
| 2:GF:708:ILE:HG13 | 2:GF:727:PHE:CE2 | 2.51 | 0.46 |
| 2:GF:938:PRO:HD2 | 2:GF:943:GLU:HB2 | 1.97 | 0.46 |
| 3:GH:217:LYS:HA | 3:GH:236:PHE:CE2 | 2.51 | 0.46 |
| 4:GI:172:GLU:OE1 | 4:GJ:164:ILE:HG23 | 2.15 | 0.46 |
| 5:HB:183:GLY:HA2 | 5:HB:307:ASN:ND2 | 2.31 | 0.46 |
| 5:HB:334:ALA:HA | 5:HB:349:TRP:NE1 | 2.31 | 0.46 |
| 5:HB:402:GLU:HG3 | 5:HB:406:LEU:HD11 | 1.96 | 0.46 |
| 5:HB:478:TRP:CH2 | 5:HB:600:ARG:HB2 | 2.50 | 0.46 |
| 5:HC:477:SER:HB2 | 5:HC:602:ALA:HB3 | 1.96 | 0.46 |
| 5:HD:275:SER:OG | 5:HD:282:VAL:HG12 | 2.16 | 0.46 |
| 7:HH:71:ASN:O | 7:HH:73:THR:HG22 | 2.16 | 0.46 |
| 7:HI:364:GLY:N | 7:HI:393:PRO:O | 2.47 | 0.46 |
| 7:HI:411:ASN:O | 7:HI:415:ASN:ND2 | 2.48 | 0.46 |
| 5:I:315:GLY:HA2 | 5:K:317:LEU:O | 2.16 | 0.46 |
| 5:I:558:ASP:N | 5:I:559:PRO:HD3 | 2.31 | 0.46 |
| 8:IB:112:ILE:HD11 | 8:IB:126:GLU:OE2 | 2.15 | 0.46 |
| 10:ID:330:ASN:O | 10:ID:339:PRO:HA | 2.16 | 0.46 |
| 5:J:460:TYR:CE2 | 5:J:462:ASN:HB2 | 2.50 | 0.46 |
| 5:J:551:ILE:HD13 | 5:K:565:ILE:CD1 | 2.46 | 0.46 |
| 5:K:310:GLU:HB2 | 5:K:384:THR:HB | 1.98 | 0.46 |
| 5:K:358:VAL:HG22 | 5:K:371:PHE:HB2 | 1.98 | 0.46 |
| 2:C:228:ARG:NH2 | 5:K:559:PRO:HB3 | 2.28 | 0.46 |
| 6:M:126:VAL:HG12 | 6:M:130:ARG:NH1 | 2.31 | 0.46 |
| 6:M:168:LEU:HB2 | 6:M:180:GLN:OE1 | 2.15 | 0.46 |
| 6:M:43:LEU:HD11 | 6:N:141:THR:HG22 | 1.97 | 0.46 |
| 7:O:101:SER:HA | 7:O:105:GLU:OE1 | 2.16 | 0.46 |
| 7:O:122:THR:HG22 | 7:O:123:VAL:H | 5.03 | 0.46 |
| 7:O:248:ALA:O | 7:O:252:GLY:N | 2.44 | 0.46 |
| 7:O:302:ILE:HD12 | 7:P:306:PHE:CZ | 2.51 | 0.46 |
| 7:O:382:ARG:HH22 | 7:O:434:VAL:HB | 1.81 | 0.46 |
| 7:P:360:ARG:HH11 | 7:P:525:VAL:HG21 | 1.81 | 0.46 |
| 8:R:112:ILE:HD11 | 8:R:126:GLU:OE2 | 2.15 | 0.46 |
| 11:V:60:ALA:HB1 | 11:V:69:LEU:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:252:LEU:HD12 | 1:X:252:LEU:O | 2.15 | 0.46 |
| 1:X:518:ASN:OD1 | 1:X:519:SER:N | 2.48 | 0.46 |
| 1:X:595:ILE:HG22 | 1:X:602:ILE:HA | 1.98 | 0.46 |
| 13:YA:121[F]:TYR:OH | 13:YA:123[F]:ARG:NH2 | 2.49 | 0.46 |
| 13:YA:180[F]:LEU:HA | 13:YA:180[F]:LEU:HD13 | 1.76 | 0.46 |
| 13:YA:257[B]:LYS:HE2 | 13:YA:266[B]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YA:321[B]:LYS:HD3 | 13:YB:452[B]:GLY:CA | 2.34 | 0.46 |
| 13:YA:416[D]:HIS:CG | 13:YA:417[D]:PRO:HD2 | 2.51 | 0.46 |
| 13:YA:490[C]:VAL:HG12 | 13:YA:492[C]:GLY:H | 1.81 | 0.46 |
| 13:YA:57[F]:VAL:HG21 | 13:YA:75[F]:GLY:HA3 | 1.98 | 0.46 |
| 13:YB:109[E]:ASN:OD1 | 13:YB:111[E]:LEU:N | 2.48 | 0.46 |
| 13:YB:121[C]:TYR:OH | 13:YB:123[C]:ARG:NH2 | 2.49 | 0.46 |
| 13:YB:146[F]:VAL:O | 13:YB:150[F]:SER:OG | 2.34 | 0.46 |
| 13:YB:39[F]:ARG:NH1 | 13:YB:113[F]:GLY:HA2 | 2.30 | 0.46 |
| 13:YB:568[B]:ASP:OD1 | 13:YB:569[B]:GLY:N | 2.49 | 0.46 |
| 13:YB:18[E]:ARG:CZ | 13:YB:77[E]:VAL:HG23 | 2.46 | 0.46 |
| 13:YB:81[D]:ARG:HB3 | 13:YB:100[D]:TYR:CZ | 2.51 | 0.46 |
| 13:YA:7[F]:ASN:ND2 | 13:YB:9[F]:ASN:HA | 2.22 | 0.46 |
| 13:YA:407[A]:PRO:HB3 | 13:YC:232[A]:ASN:CB | 2.46 | 0.46 |
| 13:YC:266[B]:TRP:CD1 | 13:YC:274[B]:GLN:HG2 | 2.51 | 0.46 |
| 13:YC:257[D]:LYS:HE2 | 13:YC:266[D]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YB:566[A]:THR:HG23 | 13:YC:558[A]:SER:HA | 1.97 | 0.46 |
| 13:YC:57[E]:VAL:HB | 13:YC:76[E]:PRO:O | 2.16 | 0.46 |
| 13:YA:34[D]:LEU:HD13 | 14:YD:163[D]:THR:HG21 | 1.97 | 0.46 |
| 14:YD:170[C]:LEU:HD23 | 14:YD:170[C]:LEU:HA | 1.69 | 0.46 |
| 14:YD:212[A]:ILE:HG22 | 14:YD:327[A]:ASN:HB2 | 1.98 | 0.46 |
| 14:YD:236[C]:TRP:CD1 | 14:YD:308[C]:ALA:HB2 | 2.51 | 0.46 |
| 14:YD:10[E]:PRO:HD2 | 14:YD:349[E]:ASN:O | 2.15 | 0.46 |
| 14:YE:117[C]:ASN:O | 14:YE:119[C]:LYS:HG3 | 2.16 | 0.46 |
| 11:DI:175:SER:HA | 14:YE:217[B]:SER:HB2 | 1.96 | 0.46 |
| 11:BF:182:ASN:ND2 | 14:YE:327[A]:ASN:HD22 | 2.14 | 0.46 |
| 14:YE:336[C]:GLU:O | 14:YE:359[C]:THR:OG1 | 2.33 | 0.46 |
| 14:YE:20[F]:TYR:HA | 14:YE:69[F]:ILE:HD12 | 1.98 | 0.46 |
| 14:YE:70[B]:ILE:N | 14:YE:88[B]:TYR:O | 2.49 | 0.46 |
| 13:YC:47[A]:ILE:HG12 | 14:YF:123[A]:PRO:HD3 | 1.97 | 0.46 |
| 13:YC:47[F]:ILE:HG12 | 14:YF:123[F]:PRO:HD3 | 1.97 | 0.46 |
| 14:YF:140[A]:TYR:CD2 | 14:YF:147[A]:THR:HA | 2.50 | 0.46 |
| 14:YF:160[D]:ILE:HG21 | 14:YF:282[D]:ALA:HB1 | 1.97 | 0.46 |
| 14:YD:95[D]:VAL:O | 14:YF:236[D]:TRP:N | 2.49 | 0.46 |
| 14:YF:70[C]:ILE:N | 14:YF:88[C]:TYR:O | 2.49 | 0.46 |
| 2:Z:314:THR:HB | 2:Z:375:VAL:HG11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:923:SER:HB3 | 2:Z:992:PRO:HG2 | 1.96 | 0.46 |
| 15:ZA:66[A]:LYS:O | 15:ZA:68[A]:TYR:HD1 | 1.99 | 0.46 |
| 15:ZA:66[D]:LYS:O | 15:ZA:68[D]:TYR:CD1 | 2.68 | 0.46 |
| 15:ZA:2[A]:SER:HB3 | 15:ZA:77[A]:MET:HB3 | 1.96 | 0.46 |
| 1:A:227:ARG:HB2 | 1:A:237:TYR:CE2 | 2.50 | 0.46 |
| 1:A:227:ARG:HB2 | 1:A:237:TYR:HE2 | 1.81 | 0.46 |
| 1:A:427:ASN:OD1 | 1:A:428:LYS:N | 2.49 | 0.46 |
| 1:A:543:THR:HG23 | 1:A:544:ASP:O | 2.15 | 0.46 |
| 5:AC:315:GLY:HA2 | 5:AE:317:LEU:O | 2.15 | 0.46 |
| 5:AD:147:LYS:O | 5:AD:147:LYS:HG3 | 2.16 | 0.46 |
| 5:AD:192:ARG:O | 5:AD:244:ILE:HA | 2.15 | 0.46 |
| 5:AD:542:LEU:HD21 | 5:AE:569:TYR:OH | 2.15 | 0.46 |
| 5:AE:340:VAL:HG22 | 6:AF:173:THR:HA | 1.98 | 0.46 |
| 5:AC:46:ALA:N | 5:AE:65:GLY:O | 2.35 | 0.46 |
| 7:AI:266:THR:HG23 | 7:AI:281:LEU:HD23 | 1.97 | 0.46 |
| 7:AI:349:TRP:NE1 | 7:AI:351:ALA:HB3 | 2.30 | 0.46 |
| 7:AI:60:ILE:HG22 | 7:AJ:52:SER:N | 2.30 | 0.46 |
| 7:AJ:347:MET:CE | 7:BA:345:ALA:HB1 | 2.45 | 0.46 |
| 7:AJ:359:TRP:CE2 | 7:AJ:524:LYS:HD3 | 2.50 | 0.46 |
| 7:BA:220:SER:OG | 7:BA:226:GLY:O | 2.33 | 0.46 |
| 7:BA:87:TYR:CZ | 7:BA:97:LEU:HD12 | 2.51 | 0.46 |
| 8:BB:135:THR:HG22 | 8:BB:156:THR:O | 2.16 | 0.46 |
| 8:BC:122:THR:HG22 | 8:BC:123:VAL:H | 1.81 | 0.46 |
| 1:BH:243:ILE:HG22 | 1:BH:258:GLY:CA | 2.45 | 0.46 |
| 2:BJ:193:MET:HB3 | 2:BJ:200:TYR:HB2 | 1.98 | 0.46 |
| 2:BJ:340:PRO:HA | 2:BJ:345:TYR:CD1 | 2.50 | 0.46 |
| 2:BJ:569:VAL:HB | 2:BJ:617:VAL:HG12 | 1.98 | 0.46 |
| 2:C:339:ASP:O | 2:C:341:LEU:N | 2.47 | 0.46 |
| 2:C:708:ILE:HG13 | 2:C:727:PHE:CE2 | 2.51 | 0.46 |
| 2:C:938:PRO:HD2 | 2:C:943:GLU:HB2 | 1.97 | 0.46 |
| 3:CA:228:ASN:O | 3:CA:231:TRP:CD1 | 2.69 | 0.46 |
| 3:CB:321:ALA:O | 3:CB:324:GLN:HB3 | 2.15 | 0.46 |
| 4:CD:200:ALA:HB3 | 4:CD:221:ILE:HD11 | 1.96 | 0.46 |
| 4:CC:63:ALA:HB3 | 4:CD:83:THR:HA | 1.98 | 0.46 |
| 4:CD:54:THR:HA | 4:CE:7:LYS:O | 2.16 | 0.46 |
| 5:CG:469:PRO:HA | 5:CG:472:TYR:CE2 | 2.51 | 0.46 |
| 5:CH:267:ASP:H | 5:CH:377:HIS:HB2 | 1.80 | 0.46 |
| 6:CI:19:GLY:N | 6:CJ:13:ARG:NH1 | 2.63 | 0.46 |
| 6:CJ:203:LEU:HD12 | 6:CJ:206:GLN:NE2 | 2.31 | 0.46 |
| 6:CJ:76:GLY:HA2 | 6:CJ:215:PHE:HZ | 1.79 | 0.46 |
| 7:DB:493:GLU:HG3 | 7:DB:496:ARG:HH21 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:77:THR:OG1 | 7:DB:78:PRO:HD2 | 2.16 | 0.46 |
| 7:DC:348:MET:SD | 7:DD:400:VAL:HG11 | 2.56 | 0.46 |
| 7:DC:31:ASP:CG | 7:DC:34:ALA:H | 2.18 | 0.46 |
| 7:DB:513:ARG:N | 7:DC:441:GLN:O | 2.35 | 0.46 |
| 7:DC:71:ASN:CG | 7:FG:365:GLY:HA2 | 2.36 | 0.46 |
| 7:DD:118:PRO:O | 7:DD:122:THR:N | 2.41 | 0.46 |
| 8:BC:117:ALA:HA | 8:DF:77:GLU:OE2 | 2.16 | 0.46 |
| 1:EA:106:ALA:HB3 | 1:EA:169:GLN:HB2 | 1.98 | 0.46 |
| 1:EA:235:GLU:C | 1:EA:236:PHE:HD1 | 2.19 | 0.46 |
| 1:EA:174:ARG:HH21 | 1:EA:269:VAL:HG21 | 1.80 | 0.46 |
| 1:EB:209:TRP:CE3 | 1:EB:212:LYS:HE3 | 2.51 | 0.46 |
| 2:EC:319:TYR:HD1 | 2:EC:328:TYR:CB | 2.29 | 0.46 |
| 2:EC:437:ASP:OD1 | 2:EC:440:LEU:HB2 | 2.16 | 0.46 |
| 2:EC:525:TRP:NE1 | 2:EC:526:ILE:O | 2.49 | 0.46 |
| 4:EG:36:ASN:OD1 | 4:EH:7:LYS:NZ | 2.29 | 0.46 |
| 5:EI:317:LEU:HD13 | 5:EJ:312:ARG:HH22 | 1.80 | 0.46 |
| 5:EI:49:TRP:HZ3 | 5:EI:96:ARG:HD2 | 1.80 | 0.46 |
| 5:EJ:313:PHE:HB3 | 5:EJ:381:ILE:HG12 | 1.98 | 0.46 |
| 4:F:63:ALA:HB3 | 4:G:83:THR:HA | 1.97 | 0.46 |
| 5:FA:267:ASP:H | 5:FA:377:HIS:HB2 | 1.80 | 0.46 |
| 6:FD:76:GLY:HA2 | 6:FD:215:PHE:HZ | 1.79 | 0.46 |
| 7:FE:99:ARG:NH1 | 7:FE:105:GLU:OE2 | 2.32 | 0.46 |
| 7:FE:160:MET:HG3 | 7:FE:164:LYS:HZ1 | 1.80 | 0.46 |
| 7:FE:342:PRO:HG2 | 7:FE:345:ALA:HB2 | 1.96 | 0.46 |
| 7:FF:31:ASP:CG | 7:FF:34:ALA:H | 2.18 | 0.46 |
| 7:FF:85:LEU:O | 7:FF:85:LEU:HD23 | 2.15 | 0.46 |
| 7:FG:220:SER:HB2 | 7:FG:228:ILE:HG12 | 1.97 | 0.46 |
| 7:FG:77:THR:HG23 | 7:FG:79:ALA:H | 1.80 | 0.46 |
| 4:G:54:THR:HA | 4:H:7:LYS:O | 2.16 | 0.46 |
| 11:GB:190:LYS:O | 11:GB:193:GLY:N | 2.48 | 0.46 |
| 12:GC:221:ILE:HA | 12:GC:221:ILE:HD12 | 1.80 | 0.46 |
| 1:GD:347:THR:O | 1:GD:351:GLU:N | 2.43 | 0.46 |
| 1:GE:506:LYS:O | 1:GE:509:SER:OG | 2.19 | 0.46 |
| 2:GF:328:TYR:H | 2:GF:353:ASP:CG | 2.19 | 0.46 |
| 2:GF:569:VAL:HB | 2:GF:617:VAL:HG12 | 1.98 | 0.46 |
| 3:GH:219:ASP:CG | 3:GH:222:ARG:H | 2.19 | 0.46 |
| 3:GH:72:TRP:HZ3 | 3:GH:275:ILE:CD1 | 2.29 | 0.46 |
| 3:GH:95:TRP:CH2 | 3:GH:169:PRO:HD3 | 2.51 | 0.46 |
| 4:GI:103:LEU:HD21 | 4:HA:113:ASN:ND2 | 2.25 | 0.46 |
| 4:GI:168:PHE:CE1 | 4:GJ:149:ARG:HB3 | 2.51 | 0.46 |
| 5:HB:289:LYS:HD2 | 5:HB:372:ASP:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:54:ALA:HB2 | 5:HB:71:ASN:O | 2.16 | 0.46 |
| 5:HC:107:VAL:O | 5:HC:125:GLU:HG3 | 2.16 | 0.46 |
| 5:HC:170:GLU:O | 5:HC:172:GLN:N | 2.48 | 0.46 |
| 5:HB:317:LEU:HD13 | 5:HC:312:ARG:HH22 | 1.80 | 0.46 |
| 5:HB:317:LEU:HD13 | 5:HC:312:ARG:NH2 | 2.30 | 0.46 |
| 5:HC:313:PHE:HE2 | 5:HC:320:LEU:HD11 | 1.80 | 0.46 |
| 5:HD:132:ASP:OD2 | 5:HD:151:ILE:HA | 2.16 | 0.46 |
| 5:HD:310:GLU:HB2 | 5:HD:384:THR:HB | 1.98 | 0.46 |
| 6:HE:203:LEU:HD12 | 6:HE:206:GLN:NE2 | 2.31 | 0.46 |
| 6:HE:141:THR:HG22 | 6:HG:43:LEU:HD11 | 1.97 | 0.46 |
| 7:HJ:127:ASN:O | 7:HJ:131:THR:HG23 | 2.15 | 0.46 |
| 7:HH:399:PHE:HD2 | 7:HJ:514:PRO:HG2 | 1.77 | 0.46 |
| 7:HJ:77:THR:HG23 | 7:HJ:79:ALA:H | 1.80 | 0.46 |
| 5:I:87:ASN:HA | 5:I:89:TYR:CE2 | 2.50 | 0.46 |
| 10:ID:207:PHE:O | 10:ID:345:GLU:HA | 2.16 | 0.46 |
| 5:J:147:LYS:HG3 | 5:J:147:LYS:O | 2.16 | 0.46 |
| 5:J:130:PHE:HB2 | 5:J:150:GLN:HB3 | 1.98 | 0.46 |
| 5:K:158:ASP:OD1 | 5:K:159:ILE:N | 2.47 | 0.46 |
| 5:K:272:SER:OG | 6:N:106:THR:N | 2.28 | 0.46 |
| 5:K:335:ASP:N | 5:K:335:ASP:OD1 | 2.47 | 0.46 |
| 6:M:71:ILE:O | 6:M:215:PHE:N | 2.36 | 0.46 |
| 6:N:126:VAL:HG12 | 6:N:130:ARG:NH1 | 2.31 | 0.46 |
| 7:O:147:LEU:HB2 | 7:O:148:PRO:HD3 | 1.98 | 0.46 |
| 7:O:231:GLY:N | 7:O:243:VAL:HB | 2.31 | 0.46 |
| 7:P:122:THR:HG22 | 7:P:123:VAL:H | 5.11 | 0.46 |
| 7:P:167:GLN:HE21 | 6:HE:77:VAL:CG2 | 2.26 | 0.46 |
| 7:P:335:ASN:H | 7:Q:329:ASN:HD21 | 1.64 | 0.46 |
| 7:P:384:GLY:O | 7:P:391:GLY:N | 2.36 | 0.46 |
| 7:P:85:LEU:O | 7:P:85:LEU:HD23 | 2.15 | 0.46 |
| 8:S:114:ARG:HD2 | 8:S:123:VAL:HG11 | 1.97 | 0.46 |
| 8:S:135:THR:HG22 | 8:S:156:THR:O | 2.16 | 0.46 |
| 1:X:444:ILE:O | 1:X:447:TYR:HB3 | 2.15 | 0.46 |
| 1:X:654:ASP:OD1 | 1:X:655:LEU:N | 2.49 | 0.46 |
| 1:Y:377:LYS:HB3 | 1:Y:377:LYS:HE2 | 1.65 | 0.46 |
| 1:Y:49:GLU:HA | 1:Y:54:ASN:ND2 | 2.28 | 0.46 |
| 13:YA:146[B]:VAL:O | 13:YA:150[B]:SER:OG | 2.34 | 0.46 |
| 13:YA:252[F]:MET:HE3 | 13:YA:252[F]:MET:HB3 | 1.84 | 0.46 |
| 13:YA:321[F]:LYS:HD3 | 13:YB:452[F]:GLY:CA | 2.34 | 0.46 |
| 13:YA:39[B]:ARG:NH1 | 13:YA:113[B]:GLY:HA2 | 2.30 | 0.46 |
| 13:YA:407[B]:PRO:HB3 | 13:YC:232[B]:ASN:CB | 2.46 | 0.46 |
| 13:YA:470[B]:ARG:HD2 | 13:YC:474[B]:ILE:HD11 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:57[E]:VAL:HB | 13:YA:76[E]:PRO:O | 2.16 | 0.46 |
| 13:YA:18[E]:ARG:CZ | 13:YA:77[E]:VAL:HG23 | 2.46 | 0.46 |
| 13:YB:116[B]:ASP:OD2 | 13:YB:121[B]:TYR:N | 2.42 | 0.46 |
| 13:YB:116[E]:ASP:OD2 | 13:YB:121[E]:TYR:N | 2.42 | 0.46 |
| 13:YB:146[E]:VAL:O | 13:YB:150[E]:SER:OG | 2.34 | 0.46 |
| 13:YB:18[D]:ARG:CZ | 13:YB:77[D]:VAL:HG23 | 2.46 | 0.46 |
| 13:YA:71[A]:GLY:HA2 | 13:YB:393[A]:MET:HA | 1.97 | 0.46 |
| 13:YB:39[D]:ARG:NH1 | 13:YB:113[D]:GLY:HA2 | 2.30 | 0.46 |
| 13:YB:416[C]:HIS:CG | 13:YB:417[C]:PRO:HD2 | 2.51 | 0.46 |
| 13:YB:416[D]:HIS:CG | 13:YB:417[D]:PRO:HD2 | 2.51 | 0.46 |
| 13:YB:492[B]:GLY:HA3 | 13:YC:485[B]:ASP:HA | 1.98 | 0.46 |
| 13:YB:567[A]:ILE:HG23 | 13:YC:565[A]:TYR:CD2 | 2.51 | 0.46 |
| 13:YC:266[C]:TRP:CD1 | 13:YC:274[C]:GLN:HG2 | 2.51 | 0.46 |
| 13:YB:315[F]:LEU:HD23 | 13:YC:367[F]:PRO:HA | 1.97 | 0.46 |
| 13:YB:69[F]:ILE:CD1 | 13:YC:396[F]:GLU:HA | 2.46 | 0.46 |
| 13:YC:416[F]:HIS:CG | 13:YC:417[F]:PRO:HD2 | 2.51 | 0.46 |
| 13:YB:481[F]:PHE:O | 13:YC:473[F]:GLN:HA | 2.15 | 0.46 |
| 13:YB:551[F]:THR:O | 13:YC:543[F]:ASP:HA | 2.16 | 0.46 |
| 13:YC:568[C]:ASP:OD1 | 13:YC:569[C]:GLY:N | 2.49 | 0.46 |
| 14:YD:160[E]:ILE:HG21 | 14:YD:282[E]:ALA:HB1 | 1.97 | 0.46 |
| 14:YD:244[F]:LYS:O | 14:YD:247[F]:PRO:HD2 | 2.14 | 0.46 |
| 14:YD:279[D]:ARG:HA | 14:YD:279[D]:ARG:HD3 | 1.43 | 0.46 |
| 14:YD:70[D]:ILE:N | 14:YD:88[D]:TYR:O | 2.49 | 0.46 |
| 14:YE:160[D]:ILE:HG21 | 14:YE:282[D]:ALA:HB1 | 1.97 | 0.46 |
| 14:YE:170[A]:LEU:HA | 14:YE:170[A]:LEU:HD23 | 1.69 | 0.46 |
| 14:YE:178[C]:LEU:CD1 | 14:YE:183[C]:ASP:HA | 2.46 | 0.46 |
| 10:U:287:VAL:O | 14:YF:100[E]:LYS:HD3 | 2.16 | 0.46 |
| 14:YF:127[C]:ASP:CG | 14:YF:130[C]:GLU:H | 2.20 | 0.46 |
| 14:YF:140[C]:TYR:CD2 | 14:YF:147[C]:THR:HA | 2.50 | 0.46 |
| 14:YF:178[A]:LEU:CD1 | 14:YF:183[A]:ASP:HA | 2.46 | 0.46 |
| 14:YF:244[B]:LYS:O | 14:YF:247[B]:PRO:HD2 | 2.14 | 0.46 |
| 13:YC:24[E]:LEU:HD23 | 14:YF:259[E]:LEU:CD2 | 2.45 | 0.46 |
| 14:YF:301[C]:MET:O | 14:YF:304[C]:TYR:N | 2.49 | 0.46 |
| 2:Z:340:PRO:HA | 2:Z:345:TYR:CD1 | 2.50 | 0.46 |
| 2:Z:360:ASN:C | 2:Z:362:LYS:N | 2.65 | 0.46 |
| 2:Z:39:ALA:HB2 | 2:Z:56:TRP:CE3 | 2.51 | 0.46 |
| 1:A:67:ILE:CD1 | 1:B:67:ILE:HG21 | 2.46 | 0.46 |
| 5:AD:313:PHE:HE2 | 5:AD:320:LEU:HD11 | 1.80 | 0.46 |
| 5:AD:313:PHE:HB3 | 5:AD:381:ILE:HG12 | 1.98 | 0.46 |
| 5:AD:469:PRO:HA | 5:AD:472:TYR:CE2 | 2.51 | 0.46 |
| 5:AE:103:ASN:O | 5:AE:104:VAL:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:1:MET:H3 | 5:AE:41:ASP:HB3 | 1.81 | 0.46 |
| 6:AF:76:GLY:HA2 | 6:AF:215:PHE:HZ | 1.79 | 0.46 |
| 6:AH:168:LEU:HB2 | 6:AH:180:GLN:OE1 | 2.15 | 0.46 |
| 7:AI:29:ILE:CG2 | 7:AI:30:THR:H | 2.18 | 0.46 |
| 7:AI:418:ASP:OD2 | 7:AJ:505:PRO:HD3 | 2.16 | 0.46 |
| 7:BA:418:ASP:OD2 | 7:BA:422:LYS:HB2 | 2.16 | 0.46 |
| 11:BF:30:ARG:NH1 | 11:BF:192:TYR:HD1 | 2.14 | 0.46 |
| 8:BB:53:PHE:HB2 | 12:BG:7:PHE:CE2 | 2.51 | 0.46 |
| 1:BH:179:TYR:HD1 | 1:BH:185:ILE:HD11 | 1.80 | 0.46 |
| 1:BH:209:TRP:CD1 | 1:BH:225:TYR:HE1 | 2.34 | 0.46 |
| 1:BI:40:GLN:HE21 | 1:BI:43:PHE:HB2 | 1.80 | 0.46 |
| 1:BI:647:ARG:HD3 | 1:BI:650:TYR:CE2 | 2.50 | 0.46 |
| 2:BJ:228:ARG:HB3 | 2:BJ:250:TYR:HB3 | 1.97 | 0.46 |
| 2:BJ:213:ASN:HB2 | 2:BJ:289:PHE:CE1 | 2.50 | 0.46 |
| 2:BJ:479:TRP:CG | 2:BJ:505:PRO:O | 2.69 | 0.46 |
| 2:BJ:525:TRP:NE1 | 2:BJ:526:ILE:O | 2.49 | 0.46 |
| 2:C:319:TYR:HD1 | 2:C:328:TYR:CB | 2.29 | 0.46 |
| 2:C:340:PRO:O | 2:C:342:SER:N | 2.46 | 0.46 |
| 2:C:573:VAL:O | 2:C:609:GLU:HA | 2.16 | 0.46 |
| 2:C:976:SER:HB2 | 5:J:10:VAL:HG21 | 1.97 | 0.46 |
| 3:CB:248:ARG:HA | 3:CB:331:LEU:HD23 | 1.97 | 0.46 |
| 3:CB:72:TRP:HZ3 | 3:CB:275:ILE:CD1 | 2.29 | 0.46 |
| 4:CC:82:GLY:O | 4:CE:64:THR:N | 2.36 | 0.46 |
| 5:CF:23:GLY:O | 5:CF:24:ILE:HB | 2.15 | 0.46 |
| 5:CF:558:ASP:N | 5:CF:559:PRO:HD3 | 2.31 | 0.46 |
| 5:CG:221:GLU:N | 5:CG:221:GLU:OE1 | 2.49 | 0.46 |
| 5:CF:182:ARG:NH1 | 5:CG:299:ILE:HG12 | 2.31 | 0.46 |
| 5:CG:322:GLY:HA2 | 5:CG:360:THR:H | 1.81 | 0.46 |
| 5:CH:22:GLY:O | 5:CH:26:ILE:HG22 | 2.16 | 0.46 |
| 5:CG:200:LEU:HD11 | 5:CH:241:THR:HG21 | 1.97 | 0.46 |
| 5:CH:289:LYS:HG3 | 5:CH:370:HIS:CE1 | 2.50 | 0.46 |
| 5:CF:315:GLY:HA2 | 5:CH:317:LEU:O | 2.16 | 0.46 |
| 6:CI:90:PHE:CD2 | 6:CI:126:VAL:HG22 | 2.45 | 0.46 |
| 6:CJ:90:PHE:CD2 | 6:CJ:126:VAL:HG22 | 2.45 | 0.46 |
| 5:CG:339:GLU:HB3 | 6:DA:172:SER:O | 2.16 | 0.46 |
| 7:DB:162:PRO:CB | 7:DC:150:ALA:HA | 2.45 | 0.46 |
| 6:AF:218:THR:HB | 7:DC:205:ARG:NH1 | 2.29 | 0.46 |
| 7:DC:347:MET:CE | 7:DD:345:ALA:HB1 | 2.45 | 0.46 |
| 8:DE:135:THR:HG22 | 8:DE:156:THR:O | 2.16 | 0.46 |
| 8:DE:14:ASP:CG | 8:DE:17:ARG:HH22 | 2.18 | 0.46 |
| 8:DF:40:ALA:O | 8:DF:69:TRP:NE1 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:DH:207:PHE:O | 10:DH:345:GLU:HA | 2.16 | 0.46 |
| 11:DI:30:ARG:NH1 | 11:DI:192:TYR:HD1 | 2.14 | 0.46 |
| 12:DJ:120:SER:HA | 12:DJ:123:LEU:HG | 1.97 | 0.46 |
| 12:DJ:196:GLU:OE2 | 12:DJ:217:THR:HG23 | 2.15 | 0.46 |
| 1:EA:200:TYR:HB2 | 1:EA:269:VAL:HG13 | 1.98 | 0.46 |
| 1:EA:544:ASP:HB2 | 1:EA:576:ASP:OD2 | 2.16 | 0.46 |
| 1:EB:209:TRP:NE1 | 1:EB:223:ILE:HG12 | 2.30 | 0.46 |
| 1:EB:200:TYR:HB2 | 1:EB:269:VAL:HG13 | 1.97 | 0.46 |
| 2:EC:193:MET:HB3 | 2:EC:200:TYR:HB2 | 1.98 | 0.46 |
| 2:EC:254:PHE:HB3 | 2:EC:294:PHE:HB3 | 1.96 | 0.46 |
| 2:EC:483:LYS:HE2 | 3:GH:241:ARG:HH12 | 1.80 | 0.46 |
| 2:EC:78:TYR:HB2 | 2:EC:100:PHE:CZ | 2.50 | 0.46 |
| 5:EI:182:ARG:HH22 | 5:EJ:299:ILE:HG21 | 1.81 | 0.46 |
| 5:EI:416:ILE:HG23 | 5:FA:472:TYR:HA | 1.98 | 0.46 |
| 5:EI:568:LYS:HB3 | 5:EJ:548:GLY:C | 2.35 | 0.46 |
| 5:EJ:30:PHE:HE1 | 5:FA:30:PHE:HE1 | 1.63 | 0.46 |
| 5:FA:344:VAL:O | 5:FA:345:LEU:HD12 | 2.16 | 0.46 |
| 6:FC:203:LEU:HD12 | 6:FC:206:GLN:NE2 | 2.31 | 0.46 |
| 7:FE:32:VAL:HA | 7:FE:35:ALA:HB3 | 1.97 | 0.46 |
| 7:FE:77:THR:OG1 | 7:FE:78:PRO:HD2 | 2.16 | 0.46 |
| 6:CI:77:VAL:CG2 | 7:FF:167:GLN:HE21 | 2.24 | 0.46 |
| 7:FF:50:ALA:HB3 | 7:FF:58:LEU:HD12 | 1.97 | 0.46 |
| 7:FF:45:ASN:CG | 7:FG:24:ASN:HD21 | 2.19 | 0.46 |
| 7:FG:383:TYR:CE1 | 7:FG:393:PRO:HG3 | 2.50 | 0.46 |
| 7:FG:418:ASP:OD2 | 7:FG:422:LYS:HB2 | 2.16 | 0.46 |
| 7:FE:504:ARG:NH2 | 7:FG:424:ARG:O | 2.47 | 0.46 |
| 7:FG:7:GLN:HB3 | 7:FG:15:TYR:CE2 | 2.51 | 0.46 |
| 11:GB:30:ARG:NH1 | 11:GB:192:TYR:HD1 | 2.14 | 0.46 |
| 11:GB:60:ALA:HB1 | 11:GB:69:LEU:O | 2.16 | 0.46 |
| 1:GD:571:PRO:HA | 1:GD:589:TYR:O | 2.15 | 0.46 |
| 1:GE:424:TYR:HE2 | 1:GE:655:LEU:HD13 | 1.81 | 0.46 |
| 1:B:430:GLN:NE2 | 2:GF:720:ARG:HD2 | 2.31 | 0.46 |
| 2:GF:737:THR:HB | 2:GF:740:ILE:HD12 | 1.98 | 0.46 |
| 2:GF:761:GLU:HB2 | 2:GF:862:TYR:CZ | 2.51 | 0.46 |
| 1:GD:341:THR:HG23 | 2:GF:880:ILE:O | 2.16 | 0.46 |
| 2:GF:977:ILE:HD13 | 5:HC:12:ASP:HB3 | 1.97 | 0.46 |
| 5:HB:129:ARG:HG3 | 5:HB:130:PHE:N | 2.30 | 0.46 |
| 5:HB:19:LEU:HD12 | 5:HB:20:ARG:N | 2.31 | 0.46 |
| 5:HB:60:LEU:CG | 5:HB:79:ILE:HG22 | 2.46 | 0.46 |
| 5:HC:120:SER:OG | 5:HC:122:VAL:HG22 | 2.16 | 0.46 |
| 5:HC:161:ASN:OD1 | 5:HC:249:ASP:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HC:186:TYR:HB3 | 5:HC:227:GLY:CA | 2.46 | 0.46 |
| 5:HC:491:ASN:ND2 | 5:HC:496:ASP:HB2 | 2.27 | 0.46 |
| 7:HI:172:LEU:O | 7:HI:175:GLN:NE2 | 2.49 | 0.46 |
| 7:HI:57:ILE:HG23 | 7:HJ:56:GLY:CA | 2.46 | 0.46 |
| 7:HJ:415:ASN:O | 7:HJ:424:ARG:HD2 | 2.16 | 0.46 |
| 7:HI:478:ASP:CG | 7:HJ:454:HIS:HE2 | 2.19 | 0.46 |
| 7:HH:469:VAL:HB | 7:HJ:477:TRP:CZ3 | 2.51 | 0.46 |
| 5:I:154:ILE:HG23 | 5:J:153:LYS:HZ1 | 1.80 | 0.46 |
| 5:I:19:LEU:HD12 | 5:I:20:ARG:N | 2.31 | 0.46 |
| 5:I:313:PHE:HE2 | 5:I:320:LEU:HD11 | 1.81 | 0.46 |
| 8:IA:22:GLN:HE21 | 8:IA:33:THR:HG21 | 1.81 | 0.46 |
| 2:GF:651:THR:HG21 | 11:IE:55:ARG:HD3 | 1.98 | 0.46 |
| 12:IF:120:SER:HA | 12:IF:123:LEU:HG | 1.97 | 0.46 |
| 5:J:3:GLN:HG3 | 5:J:25:LYS:HG3 | 1.98 | 0.46 |
| 5:J:313:PHE:HB3 | 5:J:381:ILE:HG12 | 1.98 | 0.46 |
| 5:J:359:GLU:O | 5:J:370:HIS:N | 2.45 | 0.46 |
| 5:K:344:VAL:HG12 | 5:K:349:TRP:H | 1.80 | 0.46 |
| 6:M:70:ILE:HD11 | 6:N:74:LYS:HG3 | 1.97 | 0.46 |
| 7:O:29:ILE:CG2 | 7:O:30:THR:H | 2.18 | 0.46 |
| 7:O:509:GLY:HA3 | 7:P:441:GLN:HE21 | 1.81 | 0.46 |
| 7:O:77:THR:OG1 | 7:O:78:PRO:HD2 | 2.16 | 0.46 |
| 7:P:11:ASN:N | 7:P:11:ASN:OD1 | 2.48 | 0.46 |
| 7:P:227:VAL:HG23 | 7:Q:225:LYS:HB3 | 1.98 | 0.46 |
| 7:P:216:MET:SD | 7:Q:202:GLY:HA3 | 2.55 | 0.46 |
| 7:Q:88:PRO:HG2 | 7:Q:95:TYR:O | 2.16 | 0.46 |
| 8:R:114:ARG:HD2 | 8:R:123:VAL:HG11 | 1.97 | 0.46 |
| 8:R:135:THR:HG22 | 8:R:156:THR:O | 2.16 | 0.46 |
| 1:A:52:ARG:HH21 | 9:T:25:ARG:HB3 | 1.81 | 0.46 |
| 12:W:196:GLU:OE2 | 12:W:217:THR:HG23 | 2.15 | 0.46 |
| 1:Y:209:TRP:CE3 | 1:Y:212:LYS:HE3 | 2.51 | 0.46 |
| 1:Y:23:GLY:O | 1:Y:29:ILE:HD11 | 2.15 | 0.46 |
| 1:Y:502:ASN:OD1 | 1:Y:635:ARG:NH2 | 2.48 | 0.46 |
| 13:YA:121[C]:TYR:OH | 13:YA:123[C]:ARG:NH2 | 2.49 | 0.46 |
| 13:YA:18[A]:ARG:CZ | 13:YA:77[A]:VAL:HG23 | 2.46 | 0.46 |
| 13:YA:266[F]:TRP:CD1 | 13:YA:274[F]:GLN:HG2 | 2.51 | 0.46 |
| 13:YA:498[A]:VAL:HA | 13:YB:490[A]:VAL:O | 2.16 | 0.46 |
| 13:YB:146[D]:VAL:O | 13:YB:150[D]:SER:OG | 2.34 | 0.46 |
| 13:YB:148[B]:GLN:NE2 | 13:YB:421[B]:TYR:OH | 2.48 | 0.46 |
| 13:YB:257[A]:LYS:HE2 | 13:YB:266[A]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YB:266[F]:TRP:CD1 | 13:YB:274[F]:GLN:HG2 | 2.51 | 0.46 |
| 13:YB:315[F]:LEU:O | 13:YB:319[F]:GLN:HG2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:148[F]:GLN:NE2 | 13:YB:421[F]:TYR:OH | 2.49 | 0.46 |
| 13:YB:7[E]:ASN:HD22 | 13:YB:8[E]:LEU:HG | 1.81 | 0.46 |
| 13:YB:7[F]:ASN:OD1 | 13:YC:9[F]:ASN:ND2 | 2.49 | 0.46 |
| 13:YB:67[A]:SER:HB3 | 13:YC:123[A]:ARG:HB2 | 1.98 | 0.46 |
| 13:YC:148[E]:GLN:NE2 | 13:YC:421[E]:TYR:OH | 2.48 | 0.46 |
| 13:YC:146[C]:VAL:O | 13:YC:150[C]:SER:OG | 2.34 | 0.46 |
| 13:YC:18[E]:ARG:CZ | 13:YC:77[E]:VAL:HG23 | 2.46 | 0.46 |
| 13:YB:69[D]:ILE:CD1 | 13:YC:396[D]:GLU:HA | 2.46 | 0.46 |
| 13:YC:148[C]:GLN:NE2 | 13:YC:421[C]:TYR:OH | 2.49 | 0.46 |
| 13:YA:478[D]:ASN:N | 13:YC:485[D]:ASP:O | 2.49 | 0.46 |
| 13:YC:490[E]:VAL:HG12 | 13:YC:492[E]:GLY:H | 1.81 | 0.46 |
| 13:YB:567[C]:ILE:HG23 | 13:YC:565[C]:TYR:CD2 | 2.50 | 0.46 |
| 13:YC:568[F]:ASP:OD1 | 13:YC:569[F]:GLY:N | 2.49 | 0.46 |
| 13:YC:568[D]:ASP:OD1 | 13:YC:569[D]:GLY:N | 2.49 | 0.46 |
| 13:YB:574[A]:ILE:HG22 | 13:YC:572[A]:ILE:HD13 | 1.98 | 0.46 |
| 14:YD:109[A]:LEU:HD12 | 14:YD:109[A]:LEU:HA | 1.65 | 0.46 |
| 14:YD:236[B]:TRP:CD1 | 14:YD:308[B]:ALA:HB2 | 2.51 | 0.46 |
| 14:YD:97[C]:VAL:HG12 | 14:YF:234[C]:PHE:HD1 | 1.81 | 0.46 |
| 14:YE:117[D]:ASN:O | 14:YE:119[D]:LYS:HG3 | 2.16 | 0.46 |
| 14:YE:14[D]:VAL:HG11 | 14:YE:52[D]:LEU:HD11 | 1.96 | 0.46 |
| 14:YE:160[F]:ILE:HG21 | 14:YE:282[F]:ALA:HB1 | 1.98 | 0.46 |
| 11:IE:178:ASN:HB3 | 14:YE:217[D]:SER:H | 1.81 | 0.46 |
| 14:YE:234[A]:PHE:HD1 | 14:YF:97[A]:VAL:HG12 | 1.81 | 0.46 |
| 14:YE:20[A]:TYR:HA | 14:YE:69[A]:ILE:HD12 | 1.98 | 0.46 |
| 14:YE:330[F]:LYS:HG2 | 14:YF:101[F]:GLY:HA3 | 1.98 | 0.46 |
| 14:YF:160[A]:ILE:HG21 | 14:YF:282[A]:ALA:HB1 | 1.98 | 0.46 |
| 14:YF:236[A]:TRP:CD1 | 14:YF:308[A]:ALA:HB2 | 2.51 | 0.46 |
| 14:YF:307[B]:TYR:HD1 | 14:YF:307[B]:TYR:HA | 1.66 | 0.46 |
| 14:YF:336[E]:GLU:O | 14:YF:359[E]:THR:OG1 | 2.34 | 0.46 |
| 2:Z:479:TRP:CE2 | 2:Z:505:PRO:HA | 2.50 | 0.46 |
| 2:Z:604:VAL:HG22 | 2:Z:605:ARG:H | 1.80 | 0.46 |
| 1:Y:227:ARG:NE | 2:Z:694:TYR:CZ | 2.79 | 0.46 |
| 2:Z:696:ARG:HH12 | 2:Z:726:PHE:HD1 | 1.63 | 0.46 |
| 2:Z:802:TYR:CE1 | 2:Z:807:LEU:HB3 | 2.51 | 0.46 |
| 2:Z:81:ARG:HD3 | 2:Z:96:TYR:CE1 | 2.51 | 0.46 |
| 2:Z:825:GLU:HA | 2:Z:836:GLY:O | 2.16 | 0.46 |
| 1:A:145:PHE:HD2 | 1:A:169:GLN:OE1 | 1.97 | 0.46 |
| 1:A:440:ILE:HD11 | 1:A:653:ILE:HG21 | 1.99 | 0.46 |
| 4:AA:200:ALA:HB3 | 4:AA:221:ILE:HD11 | 1.96 | 0.46 |
| 5:AC:206:PHE:CD2 | 5:AC:223:VAL:HA | 2.50 | 0.46 |
| 5:AD:126:ILE:HD12 | 5:AD:133:LEU:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:19:LEU:HD13 | 5:AE:19:LEU:HD21 | 1.98 | 0.46 |
| 5:AD:221:GLU:N | 5:AD:221:GLU:OE1 | 2.49 | 0.46 |
| 5:AD:322:GLY:HA2 | 5:AD:360:THR:H | 1.81 | 0.46 |
| 5:AE:117:ILE:HG22 | 5:AE:143:TRP:HE3 | 1.80 | 0.46 |
| 5:AE:318:GLN:HB3 | 6:AG:4:LEU:CG | 2.46 | 0.46 |
| 5:AE:372:ASP:OD1 | 5:AE:372:ASP:N | 2.48 | 0.46 |
| 6:AG:205:ASN:HB2 | 7:DC:175:GLN:O | 2.15 | 0.46 |
| 7:AI:382:ARG:HH22 | 7:AI:434:VAL:HB | 1.81 | 0.46 |
| 7:AI:405:ARG:NH2 | 7:AI:409:LEU:O | 2.49 | 0.46 |
| 7:AI:357:ASP:OD1 | 7:AJ:339:ARG:NH2 | 2.48 | 0.46 |
| 7:AJ:66:VAL:HG11 | 7:AJ:80:THR:HB | 1.98 | 0.46 |
| 1:B:491:PHE:CE2 | 1:B:619:GLN:HA | 2.51 | 0.46 |
| 7:BA:167:GLN:HG3 | 7:BA:168:LEU:HG | 1.98 | 0.46 |
| 7:AJ:478:ASP:CG | 7:BA:454:HIS:HE2 | 2.19 | 0.46 |
| 8:BB:121:LYS:HZ2 | 8:BB:122:THR:HG1 | 1.64 | 0.46 |
| 11:BF:2:LEU:N | 11:BF:2:LEU:HD12 | 2.30 | 0.46 |
| 1:BH:568:ASN:OD1 | 1:BH:569:ILE:N | 2.49 | 0.46 |
| 2:BJ:138:ASN:O | 2:BJ:555:ARG:CZ | 2.64 | 0.46 |
| 2:BJ:737:THR:HB | 2:BJ:740:ILE:HD12 | 1.98 | 0.46 |
| 2:C:1002:ALA:HA | 5:J:20:ARG:HB2 | 1.98 | 0.46 |
| 2:C:168:ILE:HA | 2:C:168:ILE:HD12 | 1.88 | 0.46 |
| 2:C:228:ARG:HB3 | 2:C:250:TYR:HB3 | 1.97 | 0.46 |
| 2:C:39:ALA:HB2 | 2:C:56:TRP:CE3 | 2.51 | 0.46 |
| 2:C:479:TRP:CE2 | 2:C:505:PRO:HA | 2.50 | 0.46 |
| 2:C:479:TRP:CG | 2:C:505:PRO:O | 2.69 | 0.46 |
| 2:C:548:ILE:N | 2:C:549:PRO:HD3 | 2.30 | 0.46 |
| 2:C:965:LEU:HG | 2:C:982:LEU:HD11 | 1.98 | 0.46 |
| 4:CD:201:LYS:NZ | 4:CD:220:ASN:OD1 | 2.37 | 0.46 |
| 4:CD:168:PHE:CE1 | 4:CE:161:ASN:HB3 | 2.50 | 0.46 |
| 5:CF:19:LEU:HD12 | 5:CF:20:ARG:N | 2.31 | 0.46 |
| 5:CF:548:GLY:O | 5:CH:568:LYS:HB3 | 2.16 | 0.46 |
| 5:CG:147:LYS:O | 5:CG:147:LYS:HG3 | 2.16 | 0.46 |
| 5:CG:265:LEU:HG | 5:CG:379:ASP:HB2 | 1.98 | 0.46 |
| 5:CG:542:LEU:HD21 | 5:CH:569:TYR:OH | 2.15 | 0.46 |
| 5:CH:102:TRP:CD1 | 5:CH:102:TRP:N | 2.83 | 0.46 |
| 5:CH:316:ILE:HD13 | 6:CJ:7:LYS:HG3 | 1.98 | 0.46 |
| 5:CF:45:SER:OG | 5:CH:66:LYS:HA | 2.16 | 0.46 |
| 7:DB:101:SER:HA | 7:DB:105:GLU:OE1 | 2.16 | 0.46 |
| 7:DB:266:THR:HG23 | 7:DB:281:LEU:HD23 | 1.97 | 0.46 |
| 7:DB:453:GLU:OE2 | 7:DB:471:THR:N | 2.32 | 0.46 |
| 7:DD:63:GLU:O | 7:DD:67:ILE:HG12 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DD:61:PRO:HD3 | 7:DD:74:LYS:HB3 | 1.97 | 0.46 |
| 8:DE:70:THR:HG22 | 8:DE:156:THR:HG22 | 1.98 | 0.46 |
| 11:DI:132:VAL:HA | 11:DI:147:GLU:HA | 1.97 | 0.46 |
| 12:DJ:195:VAL:O | 12:DJ:195:VAL:HG12 | 2.16 | 0.46 |
| 3:E:217:LYS:HA | 3:E:236:PHE:CE2 | 2.51 | 0.46 |
| 3:E:331:LEU:HD23 | 3:E:331:LEU:HA | 1.74 | 0.46 |
| 1:EA:436:LEU:O | 1:EA:439:GLN:N | 2.47 | 0.46 |
| 1:EA:642:PHE:HE1 | 1:EA:651:LEU:HD13 | 1.82 | 0.46 |
| 2:EC:314:THR:HB | 2:EC:375:VAL:HG11 | 1.98 | 0.46 |
| 3:EE:248:ARG:HA | 3:EE:331:LEU:HD23 | 1.97 | 0.46 |
| 4:EF:8:LYS:HD2 | 4:EF:30:LYS:HA | 1.98 | 0.46 |
| 5:EI:289:LYS:HD2 | 5:EI:372:ASP:HB3 | 1.98 | 0.46 |
| 5:EI:365:ILE:HB | 5:EI:366:PRO:HD2 | 1.96 | 0.46 |
| 5:EI:496:ASP:OD2 | 5:EI:499:PHE:HB2 | 2.15 | 0.46 |
| 5:FA:103:ASN:O | 5:FA:104:VAL:C | 2.54 | 0.46 |
| 6:FB:90:PHE:CD2 | 6:FB:126:VAL:HG22 | 2.45 | 0.46 |
| 6:FC:29:VAL:O | 6:FC:32:ARG:N | 2.36 | 0.46 |
| 5:FA:356:TYR:CE1 | 6:FC:4:LEU:HD13 | 2.51 | 0.46 |
| 6:FD:203:LEU:HD12 | 6:FD:206:GLN:NE2 | 2.31 | 0.46 |
| 7:FF:141:VAL:HG22 | 7:FG:139:ASN:HB2 | 1.97 | 0.46 |
| 7:FF:26:PRO:HA | 7:FF:27:PRO:HD3 | 1.72 | 0.46 |
| 7:FE:519:LEU:HA | 7:FF:434:VAL:HG13 | 1.97 | 0.46 |
| 7:FF:480:ARG:CZ | 7:FG:465:ARG:HG3 | 2.46 | 0.46 |
| 5:AD:412:PRO:HB3 | 7:FG:467:ASN:OD1 | 2.15 | 0.46 |
| 7:FG:61:PRO:HD3 | 7:FG:74:LYS:HB3 | 1.97 | 0.46 |
| 8:FH:10:PHE:CE1 | 8:IA:35:GLN:HG2 | 2.50 | 0.46 |
| 8:FI:14:ASP:CG | 8:FI:17:ARG:HH22 | 2.18 | 0.46 |
| 4:G:8:LYS:HD2 | 4:G:30:LYS:HA | 1.98 | 0.46 |
| 10:GA:323:LYS:O | 10:GA:324:THR:OG1 | 2.33 | 0.46 |
| 1:GD:243:ILE:HG22 | 1:GD:258:GLY:CA | 2.45 | 0.46 |
| 1:GD:427:ASN:OD1 | 1:GD:428:LYS:N | 2.49 | 0.46 |
| 1:GD:565:GLU:HB3 | 1:GD:570:GLN:OE1 | 2.16 | 0.46 |
| 1:GE:583:SER:OG | 1:GE:584:ASP:N | 2.49 | 0.46 |
| 2:GF:138:ASN:O | 2:GF:555:ARG:CZ | 2.64 | 0.46 |
| 2:GF:244:THR:HB | 2:GF:246:TYR:CZ | 2.51 | 0.46 |
| 2:GF:338:PHE:CE2 | 2:GF:342:SER:O | 2.69 | 0.46 |
| 2:GF:39:ALA:HB2 | 2:GF:56:TRP:CE3 | 2.51 | 0.46 |
| 2:GF:479:TRP:CG | 2:GF:505:PRO:O | 2.69 | 0.46 |
| 2:GF:548:ILE:N | 2:GF:549:PRO:HD3 | 2.30 | 0.46 |
| 2:GF:878:ASP:O | 2:GF:881:ARG:N | 2.49 | 0.46 |
| 2:GF:965:LEU:HG | 2:GF:982:LEU:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GG:310:ILE:HB | 3:GH:16:PHE:HB2 | 1.98 | 0.46 |
| 4:GJ:22:ASP:O | 4:GJ:26:ASP:N | 2.26 | 0.46 |
| 4:HA:111:ASN:HB2 | 4:HA:116:ILE:HD12 | 1.98 | 0.46 |
| 5:HB:87:ASN:HA | 5:HB:89:TYR:CE2 | 2.50 | 0.46 |
| 5:HC:190:ASN:HD22 | 5:HC:247:PHE:HD2 | 1.64 | 0.46 |
| 2:GF:1002:ALA:HA | 5:HC:20:ARG:HB2 | 1.97 | 0.46 |
| 6:HE:19:GLY:N | 6:HF:13:ARG:NH1 | 2.63 | 0.46 |
| 6:HG:86:ASP:CG | 6:HG:180:GLN:HE21 | 2.19 | 0.46 |
| 6:HG:87:TYR:N | 6:HG:181:GLU:O | 2.31 | 0.46 |
| 7:O:412:PRO:HG2 | 7:HH:87:TYR:HA | 1.97 | 0.46 |
| 7:HH:327:GLN:HG3 | 7:HJ:322:THR:O | 2.16 | 0.46 |
| 7:HJ:87:TYR:CZ | 7:HJ:97:LEU:HD12 | 2.51 | 0.46 |
| 5:I:478:TRP:CH2 | 5:I:600:ARG:HB2 | 2.50 | 0.46 |
| 5:I:54:ALA:HB2 | 5:I:71:ASN:O | 2.16 | 0.46 |
| 8:S:77:GLU:OE2 | 8:IB:117:ALA:HA | 2.16 | 0.46 |
| 8:IB:122:THR:HG22 | 8:IB:123:VAL:H | 1.81 | 0.46 |
| 11:IE:30:ARG:NH1 | 11:IE:192:TYR:HD1 | 2.14 | 0.46 |
| 11:IE:60:ALA:HB1 | 11:IE:69:LEU:O | 2.16 | 0.46 |
| 12:IF:24:CYS:CB | 12:IF:125:ILE:HD13 | 2.46 | 0.46 |
| 5:J:304:ILE:HD13 | 5:J:309:LEU:HG | 1.97 | 0.46 |
| 5:J:97:ASP:OD1 | 5:J:102:TRP:CE2 | 2.69 | 0.46 |
| 5:K:103:ASN:O | 5:K:104:VAL:C | 2.54 | 0.46 |
| 5:K:110:VAL:HG22 | 5:K:123:PRO:HB3 | 1.97 | 0.46 |
| 6:L:126:VAL:HG12 | 6:L:130:ARG:NH1 | 2.31 | 0.46 |
| 5:K:340:VAL:HG21 | 6:L:174:TYR:H | 1.81 | 0.46 |
| 8:R:79:HIS:HE1 | 8:R:151:GLN:HE22 | 1.63 | 0.46 |
| 8:S:122:THR:HG22 | 8:S:123:VAL:H | 1.81 | 0.46 |
| 1:X:544:ASP:HB2 | 1:X:576:ASP:OD2 | 2.16 | 0.46 |
| 1:Y:351:GLU:N | 1:Y:351:GLU:OE1 | 2.48 | 0.46 |
| 1:Y:485:VAL:HG11 | 1:Y:650:TYR:HE1 | 1.79 | 0.46 |
| 1:Y:491:PHE:CE2 | 1:Y:619:GLN:HA | 2.51 | 0.46 |
| 1:Y:424:TYR:HE2 | 1:Y:655:LEU:HD13 | 1.81 | 0.46 |
| 13:YA:180[A]:LEU:HA | 13:YA:180[A]:LEU:HD13 | 1.76 | 0.46 |
| 13:YA:315[B]:LEU:O | 13:YA:319[B]:GLN:HG2 | 2.16 | 0.46 |
| 13:YA:321[E]:LYS:HD3 | 13:YB:452[E]:GLY:CA | 2.34 | 0.46 |
| 13:YA:337[B]:GLU:O | 13:YA:340[B]:GLY:N | 2.48 | 0.46 |
| 13:YA:416[E]:HIS:CG | 13:YA:417[E]:PRO:HD2 | 2.51 | 0.46 |
| 13:YA:416[F]:HIS:CG | 13:YA:417[F]:PRO:HD2 | 2.51 | 0.46 |
| 13:YA:148[D]:GLN:NE2 | 13:YA:421[D]:TYR:OH | 2.48 | 0.46 |
| 13:YA:447[E]:ASN:HB3 | 13:YC:376[E]:PHE:CZ | 2.50 | 0.46 |
| 13:YA:478[F]:ASN:N | 13:YC:485[F]:ASP:O | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:574[D]:ILE:O | 15:ZA:70[D]:THR:N | 2.27 | 0.46 |
| 13:YA:66[C]:MET:HE2 | 13:YB:122[C]:PRO:HB3 | 1.98 | 0.46 |
| 13:YA:76[C]:PRO:HG3 | 13:YA:96[C]:VAL:CG1 | 2.46 | 0.46 |
| 13:YA:18[C]:ARG:CZ | 13:YA:77[C]:VAL:HG23 | 2.46 | 0.46 |
| 13:YB:121[F]:TYR:OH | 13:YB:123[F]:ARG:NH2 | 2.49 | 0.46 |
| 13:YB:18[C]:ARG:CZ | 13:YB:77[C]:VAL:HG23 | 2.46 | 0.46 |
| 13:YB:266[B]:TRP:CD1 | 13:YB:274[B]:GLN:HG2 | 2.51 | 0.46 |
| 13:YB:296[B]:LEU:HA | 13:YB:296[B]:LEU:HD12 | 1.84 | 0.46 |
| 13:YA:315[F]:LEU:HD23 | 13:YB:367[F]:PRO:HA | 1.97 | 0.46 |
| 13:YB:490[B]:VAL:HG12 | 13:YB:492[B]:GLY:H | 1.81 | 0.46 |
| 13:YB:490[C]:VAL:HG12 | 13:YB:492[C]:GLY:H | 1.81 | 0.46 |
| 13:YB:540[A]:GLY:HA3 | 13:YC:533[A]:ASN:ND2 | 2.22 | 0.46 |
| 13:YB:567[F]:ILE:HG23 | 13:YC:565[F]:TYR:CD2 | 2.50 | 0.46 |
| 13:YB:76[B]:PRO:HB2 | 13:YB:98[B]:GLY:C | 2.37 | 0.46 |
| 13:YB:57[F]:VAL:CG1 | 13:YB:76[F]:PRO:HD3 | 2.46 | 0.46 |
| 13:YB:57[E]:VAL:HB | 13:YB:76[E]:PRO:O | 2.16 | 0.46 |
| 13:YB:18[A]:ARG:CZ | 13:YB:77[A]:VAL:HG23 | 2.46 | 0.46 |
| 13:YC:39[D]:ARG:NH1 | 13:YC:113[D]:GLY:HA2 | 2.30 | 0.46 |
| 13:YC:257[E]:LYS:HE2 | 13:YC:266[E]:TRP:CZ2 | 2.50 | 0.46 |
| 13:YC:304[A]:TRP:O | 13:YC:308[A]:TYR:N | 2.32 | 0.46 |
| 13:YC:315[D]:LEU:O | 13:YC:319[D]:GLN:HG2 | 2.16 | 0.46 |
| 13:YB:70[C]:GLY:O | 13:YC:394[C]:GLU:N | 2.49 | 0.46 |
| 13:YB:69[B]:ILE:CD1 | 13:YC:396[B]:GLU:HA | 2.46 | 0.46 |
| 13:YC:416[B]:HIS:CG | 13:YC:417[B]:PRO:HD2 | 2.51 | 0.46 |
| 13:YC:57[F]:VAL:CG1 | 13:YC:76[F]:PRO:HD3 | 2.46 | 0.46 |
| 13:YC:18[A]:ARG:CZ | 13:YC:77[A]:VAL:HG23 | 2.46 | 0.46 |
| 13:YC:18[C]:ARG:CZ | 13:YC:77[C]:VAL:HG23 | 2.46 | 0.46 |
| 14:YD:127[E]:ASP:CG | 14:YD:130[E]:GLU:H | 2.20 | 0.46 |
| 14:YD:140[A]:TYR:CD2 | 14:YD:147[A]:THR:HA | 2.51 | 0.46 |
| 14:YD:160[F]:ILE:HG21 | 14:YD:282[F]:ALA:HB1 | 1.98 | 0.46 |
| 14:YD:20[A]:TYR:HA | 14:YD:69[A]:ILE:HD12 | 1.98 | 0.46 |
| 10:ID:285:LEU:HA | 14:YD:215[F]:GLU:HG3 | 1.96 | 0.46 |
| 14:YD:242[C]:PRO:HD2 | 14:YE:91[C]:LYS:O | 2.17 | 0.46 |
| 14:YD:236[E]:TRP:CD1 | 14:YD:308[E]:ALA:HB2 | 2.51 | 0.46 |
| 14:YD:236[F]:TRP:CD1 | 14:YD:308[F]:ALA:HB2 | 2.51 | 0.46 |
| 14:YD:212[E]:ILE:HG22 | 14:YD:327[E]:ASN:HB2 | 1.97 | 0.46 |
| 14:YD:38[B]:LEU:HD12 | 14:YD:38[B]:LEU:HA | 1.63 | 0.46 |
| 14:YE:127[C]:ASP:CG | 14:YE:130[C]:GLU:H | 2.20 | 0.46 |
| 14:YE:127[E]:ASP:CG | 14:YE:130[E]:GLU:H | 2.20 | 0.46 |
| 14:YE:160[C]:ILE:HG21 | 14:YE:282[C]:ALA:HB1 | 1.98 | 0.46 |
| 14:YE:244[D]:LYS:O | 14:YE:247[D]:PRO:HD2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:236[A]:TRP:CD1 | 14:YE:308[A]:ALA:HB2 | 2.51 | 0.46 |
| 14:YE:10[A]:PRO:HD2 | 14:YE:349[A]:ASN:O | 2.16 | 0.46 |
| 14:YF:109[D]:LEU:HD12 | 14:YF:109[D]:LEU:HA | 1.65 | 0.46 |
| 14:YF:236[E]:TRP:CD1 | 14:YF:308[E]:ALA:HB2 | 2.51 | 0.46 |
| 14:YF:20[B]:TYR:HA | 14:YF:69[B]:ILE:HD12 | 1.98 | 0.46 |
| 14:YF:70[E]:ILE:N | 14:YF:88[E]:TYR:O | 2.49 | 0.46 |
| 14:YE:234[E]:PHE:HD1 | 14:YF:97[E]:VAL:HG12 | 1.81 | 0.46 |
| 2:Z:525:TRP:NE1 | 2:Z:526:ILE:O | 2.49 | 0.46 |
| 2:Z:546:GLU:N | 2:Z:546:GLU:OE1 | 2.49 | 0.46 |
| 15:ZA:66[E]:LYS:O | 15:ZA:68[E]:TYR:HD1 | 1.99 | 0.46 |
| 4:AB:139:VAL:HG13 | 4:AB:164:ILE:HD12 | 1.97 | 0.45 |
| 4:AA:39:TYR:CG | 4:AB:7:LYS:HD3 | 2.51 | 0.45 |
| 5:AD:186:TYR:HB3 | 5:AD:227:GLY:CA | 2.46 | 0.45 |
| 5:AD:304:ILE:HD13 | 5:AD:309:LEU:HG | 1.97 | 0.45 |
| 5:AE:132:ASP:OD2 | 5:AE:151:ILE:HA | 2.16 | 0.45 |
| 5:AE:22:GLY:O | 5:AE:26:ILE:HG22 | 2.16 | 0.45 |
| 7:AJ:173:ILE:HD12 | 7:AJ:176:ILE:HG21 | 1.99 | 0.45 |
| 1:B:386:THR:HG23 | 1:B:387:VAL:N | 2.31 | 0.45 |
| 1:B:583:SER:OG | 1:B:584:ASP:N | 2.49 | 0.45 |
| 7:BA:101:SER:OG | 7:BA:105:GLU:HB2 | 2.17 | 0.45 |
| 7:AI:327:GLN:HG3 | 7:BA:322:THR:O | 2.16 | 0.45 |
| 7:BA:415:ASN:O | 7:BA:424:ARG:HD2 | 2.16 | 0.45 |
| 7:BA:63:GLU:O | 7:BA:67:ILE:HG12 | 2.16 | 0.45 |
| 12:BG:195:VAL:HG12 | 12:BG:195:VAL:O | 2.16 | 0.45 |
| 1:BH:236:PHE:N | 1:BH:236:PHE:CD1 | 2.84 | 0.45 |
| 1:BH:200:TYR:HB2 | 1:BH:269:VAL:HG13 | 1.98 | 0.45 |
| 1:BH:518:ASN:OD1 | 1:BH:519:SER:N | 2.48 | 0.45 |
| 1:BH:544:ASP:HB2 | 1:BH:576:ASP:OD2 | 2.16 | 0.45 |
| 1:BI:356:ILE:HG21 | 1:BI:388:GLN:NE2 | 2.30 | 0.45 |
| 1:BI:502:ASN:OD1 | 1:BI:635:ARG:NH2 | 2.48 | 0.45 |
| 2:BJ:10:SER:O | 2:BJ:25:TRP:HA | 2.16 | 0.45 |
| 2:BJ:516:TRP:HE1 | 2:BJ:518:LYS:CG | 2.29 | 0.45 |
| 2:BJ:613:LYS:O | 2:BJ:615:THR:N | 2.47 | 0.45 |
| 2:C:369:ASP:HB2 | 2:C:434:MET:HG2 | 1.99 | 0.45 |
| 2:C:825:GLU:HA | 2:C:836:GLY:O | 2.16 | 0.45 |
| 3:CA:249:PHE:O | 3:CA:329:ASN:HA | 2.16 | 0.45 |
| 3:CB:217:LYS:HA | 3:CB:236:PHE:CE2 | 2.51 | 0.45 |
| 3:CB:24:PHE:O | 3:CB:28:ILE:HD12 | 2.16 | 0.45 |
| 2:BJ:898:MET:HE1 | 3:CB:315:ARG:HH12 | 1.81 | 0.45 |
| 4:CD:67:TYR:CD1 | 4:CD:84:ARG:HB3 | 2.50 | 0.45 |
| 5:CF:10:VAL:HG23 | 5:CF:11:VAL:HG23 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:313:PHE:HE2 | 5:CF:320:LEU:HD11 | 1.80 | 0.45 |
| 5:CF:496:ASP:OD2 | 5:CF:499:PHE:HB2 | 2.15 | 0.45 |
| 5:CG:126:ILE:HD12 | 5:CG:133:LEU:HD11 | 1.98 | 0.45 |
| 5:CG:3:GLN:HG3 | 5:CG:25:LYS:HG3 | 1.98 | 0.45 |
| 5:CG:304:ILE:HD13 | 5:CG:309:LEU:HG | 1.97 | 0.45 |
| 5:CH:393:LEU:O | 5:CH:394:LEU:HB2 | 2.16 | 0.45 |
| 5:CH:563:GLY:N | 5:CH:564:PRO:HD3 | 2.31 | 0.45 |
| 6:CI:100:PRO:O | 6:CI:103:SER:OG | 2.18 | 0.45 |
| 3:D:197:ASP:OD1 | 3:D:198:VAL:N | 2.45 | 0.45 |
| 7:DB:141:VAL:HG23 | 7:DC:140:GLY:O | 2.16 | 0.45 |
| 7:DB:405:ARG:NH2 | 7:DB:409:LEU:O | 2.49 | 0.45 |
| 7:DC:11:ASN:N | 7:DC:11:ASN:OD1 | 2.48 | 0.45 |
| 7:DC:368:SER:HA | 7:DC:389:ASN:ND2 | 2.32 | 0.45 |
| 7:DD:87:TYR:CZ | 7:DD:97:LEU:HD12 | 2.51 | 0.45 |
| 8:DE:40:ALA:O | 8:DE:69:TRP:NE1 | 2.49 | 0.45 |
| 11:DI:94:TYR:CE1 | 11:DI:156:TYR:HB3 | 2.49 | 0.45 |
| 2:BJ:651:THR:HG21 | 11:DI:55:ARG:HD3 | 1.98 | 0.45 |
| 11:DI:60:ALA:HB1 | 11:DI:69:LEU:O | 2.16 | 0.45 |
| 10:DH:215:SER:O | 12:DJ:191:LEU:HD13 | 2.16 | 0.45 |
| 3:E:199:SER:OG | 3:E:200:ILE:N | 2.49 | 0.45 |
| 1:A:635:ARG:NH2 | 3:E:322:MET:SD | 2.85 | 0.45 |
| 3:E:43:ARG:NH2 | 3:E:47:TRP:CZ3 | 2.85 | 0.45 |
| 1:EA:345:TYR:OH | 1:EA:400:ASN:CG | 2.54 | 0.45 |
| 1:EB:572:TYR:HB2 | 1:EB:591:VAL:HG23 | 1.97 | 0.45 |
| 2:EC:244:THR:HB | 2:EC:246:TYR:CZ | 2.51 | 0.45 |
| 2:EC:573:VAL:O | 2:EC:609:GLU:HA | 2.16 | 0.45 |
| 2:EC:720:ARG:HD2 | 1:GE:430:GLN:NE2 | 2.32 | 0.45 |
| 3:ED:71:MET:HE1 | 3:ED:271:GLN:HG2 | 1.97 | 0.45 |
| 3:EE:17:ARG:HD2 | 3:EE:334:PHE:OXT | 2.17 | 0.45 |
| 5:EI:317:LEU:HD13 | 5:EJ:312:ARG:NH2 | 2.30 | 0.45 |
| 5:EI:334:ALA:HA | 5:EI:349:TRP:NE1 | 2.31 | 0.45 |
| 5:EI:322:GLY:HA2 | 5:EI:360:THR:H | 1.81 | 0.45 |
| 5:EJ:186:TYR:HB3 | 5:EJ:227:GLY:CA | 2.46 | 0.45 |
| 5:EJ:221:GLU:N | 5:EJ:221:GLU:OE1 | 2.49 | 0.45 |
| 5:EI:182:ARG:NH1 | 5:EJ:299:ILE:HG12 | 2.32 | 0.45 |
| 5:EJ:469:PRO:HA | 5:EJ:472:TYR:CE2 | 2.51 | 0.45 |
| 7:FE:231:GLY:N | 7:FE:243:VAL:HB | 2.31 | 0.45 |
| 7:FF:172:LEU:O | 7:FF:175:GLN:NE2 | 2.49 | 0.45 |
| 7:FF:348:MET:SD | 7:FG:400:VAL:HG11 | 2.55 | 0.45 |
| 7:FE:492:PRO:HD2 | 7:FG:464:ARG:NH2 | 2.31 | 0.45 |
| 8:FH:135:THR:HG22 | 8:FH:156:THR:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FH:46:VAL:HG13 | 8:FH:63:ASP:O | 2.16 | 0.45 |
| 1:GD:229:THR:OG1 | 1:GD:233:ASN:O | 2.35 | 0.45 |
| 1:GD:227:ARG:HB2 | 1:GD:237:TYR:HE2 | 1.81 | 0.45 |
| 1:GD:270:ILE:HG21 | 1:GD:270:ILE:HD13 | 1.69 | 0.45 |
| 1:GD:568:ASN:OD1 | 1:GD:569:ILE:N | 2.49 | 0.45 |
| 1:GD:60:LEU:HD13 | 2:GF:671:TYR:CD1 | 2.52 | 0.45 |
| 1:GD:440:ILE:HD11 | 1:GD:653:ILE:HG21 | 1.98 | 0.45 |
| 1:GE:40:GLN:HE21 | 1:GE:43:PHE:HB2 | 1.80 | 0.45 |
| 1:GE:572:TYR:HB2 | 1:GE:591:VAL:HG23 | 1.97 | 0.45 |
| 2:GF:314:THR:HB | 2:GF:375:VAL:HG11 | 1.98 | 0.45 |
| 2:GF:516:TRP:HE1 | 2:GF:518:LYS:CG | 2.29 | 0.45 |
| 3:GH:24:PHE:O | 3:GH:28:ILE:HD12 | 2.16 | 0.45 |
| 4:GJ:145:LYS:N | 4:GJ:165:GLU:O | 2.49 | 0.45 |
| 4:H:111:ASN:HB2 | 4:H:116:ILE:HD12 | 1.98 | 0.45 |
| 5:HB:10:VAL:HG23 | 5:HB:11:VAL:HG23 | 1.97 | 0.45 |
| 5:HC:358:VAL:HA | 5:HC:371:PHE:HA | 1.96 | 0.45 |
| 5:HD:267:ASP:CG | 5:HD:377:HIS:HA | 2.37 | 0.45 |
| 7:HH:382:ARG:HH22 | 7:HH:434:VAL:HB | 1.81 | 0.45 |
| 7:HH:265:LEU:N | 7:HI:256:THR:O | 2.43 | 0.45 |
| 7:HI:50:ALA:HB3 | 7:HI:58:LEU:HD12 | 1.97 | 0.45 |
| 7:HI:216:MET:SD | 7:HJ:202:GLY:HA3 | 2.55 | 0.45 |
| 7:HJ:220:SER:OG | 7:HJ:226:GLY:O | 2.33 | 0.45 |
| 5:I:183:GLY:HA2 | 5:I:307:ASN:ND2 | 2.31 | 0.45 |
| 5:I:334:ALA:HA | 5:I:349:TRP:NE1 | 2.31 | 0.45 |
| 5:I:573:LYS:HD3 | 5:J:537:THR:O | 2.16 | 0.45 |
| 5:I:60:LEU:CG | 5:I:79:ILE:HG22 | 2.46 | 0.45 |
| 8:IB:22:GLN:HE21 | 8:IB:33:THR:HG21 | 1.81 | 0.45 |
| 5:J:189:ASN:HD21 | 5:K:150:GLN:HE22 | 1.64 | 0.45 |
| 5:J:221:GLU:OE1 | 5:J:221:GLU:N | 2.49 | 0.45 |
| 5:I:317:LEU:HD13 | 5:J:312:ARG:NH1 | 2.31 | 0.45 |
| 5:J:361:ASP:H | 5:J:366:PRO:HB3 | 1.81 | 0.45 |
| 5:I:386:PHE:CZ | 5:J:390:LEU:HD13 | 2.51 | 0.45 |
| 5:K:151:ILE:HG23 | 5:K:152:ASP:H | 1.81 | 0.45 |
| 5:K:338:ASP:HB3 | 5:K:349:TRP:HD1 | 1.78 | 0.45 |
| 6:N:86:ASP:CG | 6:N:180:GLN:HE21 | 2.19 | 0.45 |
| 7:O:519:LEU:HA | 7:P:434:VAL:HG13 | 1.97 | 0.45 |
| 7:P:50:ALA:HB3 | 7:P:58:LEU:HD12 | 1.97 | 0.45 |
| 7:Q:167:GLN:HG3 | 7:Q:168:LEU:HG | 1.98 | 0.45 |
| 7:Q:221:THR:HG23 | 7:Q:223:GLU:H | 1.80 | 0.45 |
| 7:O:327:GLN:HG3 | 7:Q:322:THR:O | 2.15 | 0.45 |
| 7:O:468:PHE:HB2 | 7:Q:479:ASN:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:R:31:ASN:OD1 | 8:R:32:PHE:N | 2.48 | 0.45 |
| 8:R:40:ALA:O | 8:R:69:TRP:NE1 | 2.49 | 0.45 |
| 8:S:22:GLN:HE21 | 8:S:33:THR:HG21 | 1.81 | 0.45 |
| 10:U:221:ALA:O | 10:U:224:ASN:HB3 | 2.16 | 0.45 |
| 1:X:345:TYR:OH | 1:X:400:ASN:CG | 2.54 | 0.45 |
| 1:X:440:ILE:HD11 | 1:X:653:ILE:HG21 | 1.98 | 0.45 |
| 13:YA:81[A]:ARG:HB3 | 13:YA:100[A]:TYR:CZ | 2.51 | 0.45 |
| 13:YA:39[A]:ARG:NH1 | 13:YA:113[A]:GLY:HA2 | 2.30 | 0.45 |
| 13:YA:498[B]:VAL:HA | 13:YB:490[B]:VAL:O | 2.16 | 0.45 |
| 13:YA:534[A]:LEU:CB | 13:YC:538[A]:VAL:HG11 | 2.47 | 0.45 |
| 13:YA:558[D]:SER:O | 13:YB:551[D]:THR:HA | 2.16 | 0.45 |
| 13:YA:57[F]:VAL:CG1 | 13:YA:76[F]:PRO:HD3 | 2.46 | 0.45 |
| 13:YA:61[C]:ILE:HG13 | 13:YA:62[C]:THR:N | 2.27 | 0.45 |
| 13:YB:39[E]:ARG:NH1 | 13:YB:113[E]:GLY:HA2 | 2.30 | 0.45 |
| 13:YB:416[B]:HIS:CG | 13:YB:417[B]:PRO:HD2 | 2.51 | 0.45 |
| 13:YB:148[A]:GLN:NE2 | 13:YB:421[A]:TYR:OH | 2.48 | 0.45 |
| 13:YB:490[A]:VAL:HG12 | 13:YB:492[A]:GLY:H | 1.82 | 0.45 |
| 13:YB:568[E]:ASP:OD1 | 13:YB:569[E]:GLY:N | 2.49 | 0.45 |
| 13:YC:39[C]:ARG:NH1 | 13:YC:113[C]:GLY:HA2 | 2.30 | 0.45 |
| 13:YA:452[B]:GLY:CA | 13:YC:321[B]:LYS:HD3 | 2.40 | 0.45 |
| 13:YC:337[D]:GLU:O | 13:YC:340[D]:GLY:N | 2.48 | 0.45 |
| 13:YA:60[B]:PRO:CD | 13:YC:61[B]:ILE:HG12 | 2.46 | 0.45 |
| 10:GA:285:LEU:HA | 14:YD:215[E]:GLU:HG3 | 1.97 | 0.45 |
| 14:YD:10[C]:PRO:HD2 | 14:YD:349[C]:ASN:O | 2.16 | 0.45 |
| 14:YD:10[F]:PRO:HD2 | 14:YD:349[F]:ASN:O | 2.16 | 0.45 |
| 14:YD:20[F]:TYR:HA | 14:YD:69[F]:ILE:HD12 | 1.98 | 0.45 |
| 14:YE:117[B]:ASN:O | 14:YE:119[B]:LYS:HG3 | 2.16 | 0.45 |
| 14:YE:170[D]:LEU:HA | 14:YE:170[D]:LEU:HD23 | 1.68 | 0.45 |
| 14:YE:178[F]:LEU:CD1 | 14:YE:183[F]:ASP:HA | 2.45 | 0.45 |
| 14:YE:236[D]:TRP:CD1 | 14:YE:308[D]:ALA:HB2 | 2.51 | 0.45 |
| 14:YE:236[E]:TRP:N | 14:YF:95[E]:VAL:O | 2.48 | 0.45 |
| 14:YE:212[B]:ILE:HG22 | 14:YE:327[B]:ASN:HB2 | 1.97 | 0.45 |
| 14:YE:73[B]:SER:HB2 | 14:YE:85[B]:THR:HG23 | 1.99 | 0.45 |
| 14:YE:70[A]:ILE:N | 14:YE:88[A]:TYR:O | 2.49 | 0.45 |
| 14:YF:135[D]:MET:SD | 14:YF:166[D]:PHE:HD1 | 2.39 | 0.45 |
| 14:YF:178[D]:LEU:CD1 | 14:YF:183[D]:ASP:HA | 2.45 | 0.45 |
| 11:IE:175:SER:HA | 14:YF:217[B]:SER:HB2 | 1.97 | 0.45 |
| 11:DI:182:ASN:ND2 | 14:YF:327[F]:ASN:HD22 | 2.14 | 0.45 |
| 14:YD:61[D]:HIS:NE2 | 14:YF:332[D]:GLN:HB3 | 2.31 | 0.45 |
| 14:YF:38[D]:LEU:HD12 | 14:YF:38[D]:LEU:HA | 1.63 | 0.45 |
| 14:YF:20[A]:TYR:HA | 14:YF:69[A]:ILE:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:209:VAL:O | 2:Z:221:ALA:HA | 2.16 | 0.45 |
| 2:Z:347:GLU:CG | 2:Z:349:LEU:HD21 | 2.46 | 0.45 |
| 2:Z:516:TRP:HE1 | 2:Z:518:LYS:CG | 2.29 | 0.45 |
| 2:Z:541:TYR:CG | 2:Z:542:THR:N | 2.85 | 0.45 |
| 2:Z:938:PRO:HD2 | 2:Z:943:GLU:HB2 | 1.97 | 0.45 |
| 1:A:448:TYR:C | 1:A:453:GLU:HG2 | 2.37 | 0.45 |
| 5:AC:214:SER:HB2 | 5:AC:215:PRO:HD2 | 1.98 | 0.45 |
| 5:AC:317:LEU:HD13 | 5:AD:312:ARG:HH22 | 1.81 | 0.45 |
| 5:AE:267:ASP:CG | 5:AE:377:HIS:HA | 2.37 | 0.45 |
| 5:AE:275:SER:OG | 5:AE:282:VAL:HG12 | 2.16 | 0.45 |
| 5:AE:265:LEU:HB3 | 5:AE:281:TYR:HB3 | 1.99 | 0.45 |
| 5:AD:339:GLU:HB3 | 6:AH:172:SER:O | 2.16 | 0.45 |
| 7:AI:71:ASN:O | 7:AI:73:THR:HG22 | 2.16 | 0.45 |
| 7:AJ:368:SER:HA | 7:AJ:389:ASN:ND2 | 2.32 | 0.45 |
| 7:AJ:418:ASP:HA | 7:AJ:424:ARG:NH2 | 2.32 | 0.45 |
| 1:B:121:ASN:HA | 1:B:155:ARG:HD3 | 1.99 | 0.45 |
| 1:B:182:LEU:O | 1:B:182:LEU:HD12 | 2.16 | 0.45 |
| 1:B:200:TYR:HB2 | 1:B:269:VAL:HG13 | 1.97 | 0.45 |
| 7:AI:138:SER:C | 7:BA:143:LYS:HG2 | 2.36 | 0.45 |
| 11:BF:64:TYR:OH | 11:BF:172:ILE:O | 2.30 | 0.45 |
| 11:BF:5:PHE:CE2 | 11:BF:188:MET:HG2 | 2.52 | 0.45 |
| 12:BG:14:ALA:O | 12:DJ:166:SER:HB2 | 2.16 | 0.45 |
| 12:BG:196:GLU:OE2 | 12:BG:217:THR:HG23 | 2.15 | 0.45 |
| 1:BH:229:THR:OG1 | 1:BH:233:ASN:O | 2.35 | 0.45 |
| 1:BI:182:LEU:O | 1:BI:182:LEU:HD12 | 2.16 | 0.45 |
| 1:BI:73:ALA:O | 1:BI:77:GLU:HB2 | 2.16 | 0.45 |
| 2:BJ:314:THR:HB | 2:BJ:375:VAL:HG11 | 1.98 | 0.45 |
| 2:BJ:525:TRP:CE2 | 2:BJ:526:ILE:O | 2.68 | 0.45 |
| 2:BJ:629:GLU:OE1 | 2:BJ:629:GLU:N | 2.40 | 0.45 |
| 1:BI:227:ARG:NE | 2:BJ:694:TYR:CZ | 2.81 | 0.45 |
| 2:BJ:708:ILE:HG13 | 2:BJ:727:PHE:CE2 | 2.51 | 0.45 |
| 2:C:737:THR:HB | 2:C:740:ILE:HD12 | 1.98 | 0.45 |
| 2:C:748:PHE:CD2 | 2:C:756:VAL:HG11 | 2.52 | 0.45 |
| 2:C:802:TYR:CE1 | 2:C:807:LEU:HB3 | 2.51 | 0.45 |
| 2:C:878:ASP:O | 2:C:881:ARG:N | 2.49 | 0.45 |
| 3:CA:93:ARG:HH21 | 3:CA:106:PHE:HD1 | 1.64 | 0.45 |
| 3:CB:204:THR:O | 3:CB:207:TYR:N | 2.49 | 0.45 |
| 5:CF:272:SER:OG | 6:CI:106:THR:N | 2.49 | 0.45 |
| 5:CF:290:SER:N | 5:CF:371:PHE:O | 2.49 | 0.45 |
| 5:CF:312:ARG:HG2 | 5:CF:317:LEU:CA | 2.44 | 0.45 |
| 5:CF:87:ASN:HA | 5:CF:89:TYR:CE2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:97:ASP:OD1 | 5:CG:102:TRP:CE2 | 2.68 | 0.45 |
| 3:D:92:ARG:NH1 | 3:D:94:ASP:OD2 | 2.44 | 0.45 |
| 7:DB:231:GLY:N | 7:DB:243:VAL:HB | 2.31 | 0.45 |
| 7:DB:415:ASN:O | 7:DB:424:ARG:HD2 | 2.17 | 0.45 |
| 7:DB:139:ASN:N | 7:DD:143:LYS:HG2 | 2.31 | 0.45 |
| 11:DI:14:LYS:O | 11:DI:15:THR:HG22 | 2.17 | 0.45 |
| 1:EA:102:SER:OG | 1:EA:103:LYS:N | 2.48 | 0.45 |
| 1:EA:270:ILE:HD13 | 1:EA:270:ILE:HG21 | 1.69 | 0.45 |
| 1:EB:106:ALA:HB2 | 1:EB:280:ALA:CB | 2.45 | 0.45 |
| 1:EB:349:VAL:HG13 | 1:EB:392:ILE:HD11 | 1.98 | 0.45 |
| 1:EB:73:ALA:O | 1:EB:77:GLU:HB2 | 2.16 | 0.45 |
| 2:EC:202:PHE:HB3 | 2:EC:209:VAL:HG22 | 1.99 | 0.45 |
| 3:ED:257:TYR:HB3 | 3:ED:296:TYR:CE2 | 2.50 | 0.45 |
| 3:EE:199:SER:OG | 3:EE:200:ILE:N | 2.49 | 0.45 |
| 3:EE:43:ARG:NH2 | 3:EE:47:TRP:CZ3 | 2.85 | 0.45 |
| 4:EF:22:ASP:O | 4:EF:26:ASP:N | 2.26 | 0.45 |
| 4:EF:7:LYS:HB3 | 4:EH:53:GLY:O | 2.16 | 0.45 |
| 5:EI:290:SER:N | 5:EI:371:PHE:O | 2.49 | 0.45 |
| 5:EI:60:LEU:CG | 5:EI:79:ILE:HG22 | 2.46 | 0.45 |
| 5:EJ:261:ARG:N | 5:EJ:383:ILE:O | 2.35 | 0.45 |
| 5:EJ:36:GLU:HA | 5:EJ:50:LYS:HZ1 | 1.80 | 0.45 |
| 5:EJ:255:ARG:HH21 | 5:FA:249:ASP:HB2 | 1.81 | 0.45 |
| 5:FA:304:ILE:HD11 | 5:FA:366:PRO:HG3 | 1.99 | 0.45 |
| 5:EI:418:GLY:C | 5:FA:472:TYR:HB3 | 2.37 | 0.45 |
| 6:FD:126:VAL:HG12 | 6:FD:130:ARG:NH1 | 2.31 | 0.45 |
| 7:FE:125:LEU:O | 7:FE:129:PHE:N | 2.45 | 0.45 |
| 7:FE:248:ALA:O | 7:FE:252:GLY:N | 2.44 | 0.45 |
| 7:FF:165:THR:HA | 7:FF:168:LEU:HB2 | 1.98 | 0.45 |
| 7:FE:485:ASN:C | 7:FF:446:LYS:HG2 | 2.36 | 0.45 |
| 7:FG:335:ASN:OD1 | 7:FG:336:GLU:N | 2.47 | 0.45 |
| 8:FI:22:GLN:HE21 | 8:FI:33:THR:HG21 | 1.81 | 0.45 |
| 8:FI:40:ALA:O | 8:FI:69:TRP:NE1 | 2.49 | 0.45 |
| 10:GA:207:PHE:O | 10:GA:345:GLU:HA | 2.16 | 0.45 |
| 1:GE:121:ASN:HA | 1:GE:155:ARG:HD3 | 1.99 | 0.45 |
| 1:GE:348:PHE:HZ | 1:GE:399:TYR:CD2 | 2.35 | 0.45 |
| 1:GE:73:ALA:O | 1:GE:77:GLU:HB2 | 2.16 | 0.45 |
| 2:GF:356:THR:OG1 | 2:GF:357:ILE:O | 2.21 | 0.45 |
| 4:GI:61:ILE:O | 4:GJ:4:GLN:NE2 | 2.44 | 0.45 |
| 4:H:178:THR:HA | 4:H:275:ALA:HA | 1.97 | 0.45 |
| 5:HC:304:ILE:HD13 | 5:HC:309:LEU:HG | 1.97 | 0.45 |
| 5:HB:591:PRO:HD3 | 5:HC:522:SER:C | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:22:GLY:O | 5:HD:26:ILE:HG22 | 2.16 | 0.45 |
| 5:HD:163:ALA:O | 5:HD:246:THR:HG22 | 2.16 | 0.45 |
| 5:HC:569:TYR:HD1 | 5:HD:544:VAL:HA | 1.80 | 0.45 |
| 5:HD:71:ASN:OD1 | 5:HD:73:SER:N | 2.32 | 0.45 |
| 7:HH:101:SER:HA | 7:HH:105:GLU:OE1 | 2.16 | 0.45 |
| 7:HH:231:GLY:H | 7:HH:243:VAL:HB | 1.82 | 0.45 |
| 7:HH:231:GLY:N | 7:HH:243:VAL:HB | 2.31 | 0.45 |
| 7:HI:360:ARG:HH11 | 7:HI:525:VAL:HG21 | 1.80 | 0.45 |
| 7:HI:59:PHE:CZ | 7:HJ:55:LYS:HG3 | 2.52 | 0.45 |
| 7:HJ:7:GLN:HB3 | 7:HJ:15:TYR:CE2 | 2.51 | 0.45 |
| 7:HJ:221:THR:HG23 | 7:HJ:223:GLU:H | 1.80 | 0.45 |
| 7:HJ:418:ASP:OD2 | 7:HJ:422:LYS:HB2 | 2.16 | 0.45 |
| 5:K:186:TYR:HD2 | 5:K:227:GLY:HA2 | 1.80 | 0.45 |
| 5:K:202:TYR:CE1 | 5:K:206:PHE:HD1 | 2.35 | 0.45 |
| 5:K:163:ALA:O | 5:K:246:THR:HG22 | 2.16 | 0.45 |
| 5:K:393:LEU:O | 5:K:394:LEU:HB2 | 2.16 | 0.45 |
| 5:K:36:GLU:HA | 5:K:50:LYS:HZ1 | 1.82 | 0.45 |
| 5:I:45:SER:OG | 5:K:66:LYS:HA | 2.17 | 0.45 |
| 7:O:160:MET:HA | 7:O:164:LYS:HZ1 | 1.81 | 0.45 |
| 7:O:301:ARG:O | 7:Q:295:ILE:HA | 2.16 | 0.45 |
| 7:O:415:ASN:O | 7:O:424:ARG:HD2 | 2.17 | 0.45 |
| 7:P:170:ILE:HG23 | 7:Q:173:ILE:HD13 | 1.98 | 0.45 |
| 7:P:364:GLY:N | 7:P:393:PRO:O | 2.47 | 0.45 |
| 7:O:43:GLY:HA3 | 7:P:39:ILE:HG23 | 1.98 | 0.45 |
| 7:P:458:GLY:O | 7:P:461:GLY:N | 2.41 | 0.45 |
| 7:Q:220:SER:OG | 7:Q:226:GLY:O | 2.33 | 0.45 |
| 7:O:469:VAL:HB | 7:Q:477:TRP:CZ3 | 2.50 | 0.45 |
| 8:R:22:GLN:HE21 | 8:R:33:THR:HG21 | 1.81 | 0.45 |
| 8:R:70:THR:HG22 | 8:R:156:THR:HG22 | 1.97 | 0.45 |
| 1:X:227:ARG:HB2 | 1:X:237:TYR:HE2 | 1.81 | 0.45 |
| 1:X:554:ILE:HG22 | 1:X:555:ILE:O | 2.16 | 0.45 |
| 13:YA:148[F]:GLN:NE2 | 13:YA:421[F]:TYR:OH | 2.49 | 0.45 |
| 13:YA:252[B]:MET:HB3 | 13:YA:252[B]:MET:HE3 | 1.80 | 0.45 |
| 13:YA:393[C]:MET:HA | 13:YC:71[C]:GLY:HA2 | 1.99 | 0.45 |
| 13:YA:416[A]:HIS:CG | 13:YA:417[A]:PRO:HD2 | 2.51 | 0.45 |
| 13:YA:490[D]:VAL:HG12 | 13:YA:492[D]:GLY:H | 1.82 | 0.45 |
| 13:YA:490[E]:VAL:HG12 | 13:YA:492[E]:GLY:H | 1.81 | 0.45 |
| 13:YA:558[F]:SER:O | 13:YB:551[F]:THR:HA | 2.16 | 0.45 |
| 13:YA:568[D]:ASP:OD1 | 13:YA:569[D]:GLY:N | 2.49 | 0.45 |
| 13:YA:568[F]:ASP:OD1 | 13:YA:569[F]:GLY:N | 2.49 | 0.45 |
| 13:YB:551[B]:THR:O | 13:YC:543[B]:ASP:HA | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:552[E]:GLU:HB2 | 13:YC:544[E]:TRP:HB2 | 1.98 | 0.45 |
| 13:YB:552[F]:GLU:HB2 | 13:YC:544[F]:TRP:HB2 | 1.98 | 0.45 |
| 13:YB:71[A]:GLY:HA2 | 13:YC:393[A]:MET:HA | 1.98 | 0.45 |
| 13:YB:18[F]:ARG:CZ | 13:YB:77[F]:VAL:HG23 | 2.45 | 0.45 |
| 13:YB:7[C]:ASN:OD1 | 13:YC:9[C]:ASN:ND2 | 2.49 | 0.45 |
| 13:YC:18[F]:ARG:CZ | 13:YC:77[F]:VAL:HG23 | 2.45 | 0.45 |
| 13:YC:416[C]:HIS:CG | 13:YC:417[C]:PRO:HD2 | 2.51 | 0.45 |
| 13:YC:568[B]:ASP:OD1 | 13:YC:569[B]:GLY:N | 2.49 | 0.45 |
| 13:YB:574[E]:ILE:HG22 | 13:YC:572[E]:ILE:HD13 | 1.97 | 0.45 |
| 14:YD:10[B]:PRO:HD2 | 14:YD:349[B]:ASN:O | 2.17 | 0.45 |
| 14:YD:117[F]:ASN:O | 14:YD:119[F]:LYS:HG3 | 2.17 | 0.45 |
| 14:YD:117[B]:ASN:O | 14:YD:119[B]:LYS:HG3 | 2.16 | 0.45 |
| 14:YD:127[A]:ASP:CG | 14:YD:130[A]:GLU:H | 2.20 | 0.45 |
| 14:YD:178[B]:LEU:CD1 | 14:YD:183[B]:ASP:HA | 2.45 | 0.45 |
| 14:YD:330[B]:LYS:HG2 | 14:YE:101[B]:GLY:HA3 | 1.98 | 0.45 |
| 14:YD:336[B]:GLU:O | 14:YD:359[B]:THR:OG1 | 2.33 | 0.45 |
| 14:YD:336[E]:GLU:O | 14:YD:359[E]:THR:OG1 | 2.34 | 0.45 |
| 14:YD:70[C]:ILE:N | 14:YD:88[C]:TYR:O | 2.49 | 0.45 |
| 14:YD:97[A]:VAL:HG12 | 14:YF:234[A]:PHE:HD1 | 1.80 | 0.45 |
| 14:YE:109[E]:LEU:HA | 14:YE:109[E]:LEU:HD12 | 1.65 | 0.45 |
| 14:YE:212[C]:ILE:HG22 | 14:YE:327[C]:ASN:HB2 | 1.97 | 0.45 |
| 14:YE:212[F]:ILE:HG22 | 14:YE:327[F]:ASN:HB2 | 1.97 | 0.45 |
| 10:DH:285:LEU:HA | 14:YE:215[B]:GLU:CG | 2.45 | 0.45 |
| 14:YE:236[F]:TRP:CD1 | 14:YE:308[F]:ALA:HB2 | 2.51 | 0.45 |
| 14:YE:330[D]:LYS:HG2 | 14:YF:101[D]:GLY:HA3 | 1.99 | 0.45 |
| 14:YE:336[E]:GLU:O | 14:YE:359[E]:THR:OG1 | 2.34 | 0.45 |
| 14:YF:109[C]:LEU:HA | 14:YF:109[C]:LEU:HD12 | 1.65 | 0.45 |
| 13:YC:47[B]:ILE:HG12 | 14:YF:123[B]:PRO:HD3 | 1.98 | 0.45 |
| 14:YF:140[D]:TYR:CD2 | 14:YF:147[D]:THR:HA | 2.50 | 0.45 |
| 14:YF:160[E]:ILE:HG21 | 14:YF:282[E]:ALA:HB1 | 1.97 | 0.45 |
| 14:YF:266[B]:ILE:HD11 | 14:YF:290[B]:ASN:CG | 2.36 | 0.45 |
| 14:YF:20[C]:TYR:HA | 14:YF:69[C]:ILE:HD12 | 1.98 | 0.45 |
| 2:Z:319:TYR:HD1 | 2:Z:328:TYR:CB | 2.29 | 0.45 |
| 2:Z:328:TYR:H | 2:Z:353:ASP:CG | 2.19 | 0.45 |
| 2:Z:629:GLU:N | 2:Z:629:GLU:OE1 | 2.40 | 0.45 |
| 2:Z:706:SER:O | 2:Z:708:ILE:N | 2.42 | 0.45 |
| 2:Z:748:PHE:CD2 | 2:Z:756:VAL:HG11 | 2.52 | 0.45 |
| 1:A:229:THR:OG1 | 1:A:233:ASN:O | 2.35 | 0.45 |
| 4:AA:111:ASN:HB2 | 4:AA:116:ILE:HD12 | 1.98 | 0.45 |
| 5:AC:49:TRP:HB2 | 5:AE:90:ASN:OD1 | 2.17 | 0.45 |
| 5:AC:548:GLY:O | 5:AE:568:LYS:HB3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:558:ASP:N | 5:AC:559:PRO:HD3 | 2.31 | 0.45 |
| 5:AC:317:LEU:HD13 | 5:AD:312:ARG:NH2 | 2.31 | 0.45 |
| 5:AE:563:GLY:N | 5:AE:564:PRO:HD3 | 2.31 | 0.45 |
| 6:AF:19:GLY:H | 6:AG:13:ARG:CZ | 2.28 | 0.45 |
| 6:AF:73:ASN:HB3 | 6:AH:69:THR:HA | 1.99 | 0.45 |
| 6:AH:71:ILE:O | 6:AH:215:PHE:N | 2.36 | 0.45 |
| 7:AI:231:GLY:N | 7:AI:243:VAL:HB | 2.31 | 0.45 |
| 7:AI:231:GLY:H | 7:AI:243:VAL:HB | 1.81 | 0.45 |
| 7:AI:283:TRP:CZ3 | 7:AI:284:ASN:HB3 | 2.52 | 0.45 |
| 7:AJ:172:LEU:O | 7:AJ:175:GLN:NE2 | 2.49 | 0.45 |
| 1:B:73:ALA:O | 1:B:77:GLU:HB2 | 2.16 | 0.45 |
| 7:BA:67:ILE:HA | 7:BA:84:ARG:NH2 | 2.31 | 0.45 |
| 8:BC:135:THR:HG22 | 8:BC:156:THR:O | 2.16 | 0.45 |
| 8:BB:3:VAL:HG21 | 8:BC:56:ARG:NH2 | 2.31 | 0.45 |
| 11:BF:132:VAL:HA | 11:BF:147:GLU:HA | 1.97 | 0.45 |
| 1:BH:427:ASN:OD1 | 1:BH:428:LYS:N | 2.49 | 0.45 |
| 1:BH:448:TYR:C | 1:BH:453:GLU:HG2 | 2.37 | 0.45 |
| 1:BH:543:THR:HG23 | 1:BH:544:ASP:O | 2.15 | 0.45 |
| 1:BI:424:TYR:HE2 | 1:BI:655:LEU:HD13 | 1.81 | 0.45 |
| 2:BJ:808:GLN:HE21 | 2:BJ:839:ILE:HG13 | 1.80 | 0.45 |
| 1:B:50:GLY:HA2 | 2:C:657:TYR:OH | 2.17 | 0.45 |
| 2:C:664:PHE:HB2 | 9:T:15:MET:CB | 2.42 | 0.45 |
| 3:CB:43:ARG:NH2 | 3:CB:47:TRP:CZ3 | 2.84 | 0.45 |
| 4:CC:8:LYS:HD2 | 4:CC:30:LYS:HA | 1.98 | 0.45 |
| 4:CD:111:ASN:HB2 | 4:CD:116:ILE:HD12 | 1.98 | 0.45 |
| 5:CG:260:ARG:HA | 5:CG:384:THR:HA | 1.98 | 0.45 |
| 5:CG:503:ASN:OD1 | 5:CG:504:ASN:N | 2.49 | 0.45 |
| 5:CH:115:ASP:OD2 | 5:CH:137:TYR:HE1 | 2.00 | 0.45 |
| 5:CG:249:ASP:CA | 5:CH:158:ASP:HB3 | 2.46 | 0.45 |
| 5:CH:267:ASP:CG | 5:CH:377:HIS:HA | 2.37 | 0.45 |
| 6:CJ:126:VAL:HG12 | 6:CJ:130:ARG:NH1 | 2.31 | 0.45 |
| 3:D:59:PRO:HB2 | 2:GF:473:TYR:HB2 | 1.98 | 0.45 |
| 3:D:64:SER:OG | 3:D:67:GLY:N | 2.36 | 0.45 |
| 7:DB:147:LEU:HB2 | 7:DB:148:PRO:HD3 | 1.97 | 0.45 |
| 7:DB:349:TRP:NE1 | 7:DB:353:SER:O | 2.50 | 0.45 |
| 7:DC:170:ILE:HG23 | 7:DD:173:ILE:HD13 | 1.98 | 0.45 |
| 8:DF:135:THR:HG22 | 8:DF:156:THR:O | 2.16 | 0.45 |
| 12:DJ:127:SER:HB3 | 12:DJ:161:SER:HG | 1.81 | 0.45 |
| 1:EA:448:TYR:C | 1:EA:453:GLU:HG2 | 2.37 | 0.45 |
| 1:EA:510:MET:HE3 | 1:EA:623:LEU:HD11 | 1.98 | 0.45 |
| 1:EB:538:VAL:HG11 | 1:EB:558:PHE:HE1 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:634:THR:HB | 1:EB:638:SER:O | 2.17 | 0.45 |
| 2:EC:39:ALA:HB2 | 2:EC:56:TRP:CE3 | 2.51 | 0.45 |
| 2:EC:146:LEU:HD11 | 2:EC:578:PHE:CE1 | 2.51 | 0.45 |
| 2:EC:825:GLU:HA | 2:EC:836:GLY:O | 2.16 | 0.45 |
| 3:ED:174:GLY:HA3 | 3:ED:180:ILE:HG12 | 1.97 | 0.45 |
| 3:EE:72:TRP:HZ3 | 3:EE:275:ILE:CD1 | 2.29 | 0.45 |
| 4:EF:161:ASN:HB3 | 4:EH:168:PHE:CE1 | 2.51 | 0.45 |
| 5:EI:10:VAL:HG23 | 5:EI:11:VAL:HG23 | 1.97 | 0.45 |
| 5:EI:160:SER:HB3 | 5:EJ:161:ASN:ND2 | 2.22 | 0.45 |
| 5:EI:323:THR:HG21 | 5:EI:354:THR:HG23 | 1.98 | 0.45 |
| 5:EI:486:VAL:HG12 | 5:EJ:488:VAL:HG22 | 1.98 | 0.45 |
| 5:EJ:126:ILE:HD12 | 5:EJ:133:LEU:HD11 | 1.98 | 0.45 |
| 5:EJ:147:LYS:O | 5:EJ:147:LYS:HG3 | 2.16 | 0.45 |
| 5:EJ:265:LEU:HG | 5:EJ:379:ASP:HB2 | 1.98 | 0.45 |
| 5:FA:137:TYR:HD1 | 5:FA:143:TRP:HE1 | 1.61 | 0.45 |
| 5:FA:157:SER:O | 5:FA:160:SER:OG | 2.28 | 0.45 |
| 5:EJ:11:VAL:HG13 | 5:FA:20:ARG:HG2 | 1.98 | 0.45 |
| 7:FE:71:ASN:O | 7:FE:73:THR:HG22 | 2.16 | 0.45 |
| 7:FF:368:SER:HA | 7:FF:389:ASN:ND2 | 2.32 | 0.45 |
| 7:FF:40:SER:HB3 | 7:FG:24:ASN:CB | 2.44 | 0.45 |
| 7:FE:257:THR:HA | 7:FG:265:LEU:O | 2.16 | 0.45 |
| 7:FF:347:MET:CE | 7:FG:345:ALA:HB1 | 2.46 | 0.45 |
| 10:GA:203:ARG:NH2 | 10:GA:356:ARG:HH12 | 2.13 | 0.45 |
| 1:GD:106:ALA:HB3 | 1:GD:169:GLN:HB2 | 1.98 | 0.45 |
| 1:GD:654:ASP:OD1 | 1:GD:655:LEU:N | 2.49 | 0.45 |
| 3:GH:43:ARG:NH2 | 3:GH:47:TRP:CZ3 | 2.85 | 0.45 |
| 5:HB:386:PHE:CZ | 5:HC:390:LEU:HD13 | 2.51 | 0.45 |
| 5:HC:469:PRO:HA | 5:HC:472:TYR:CE2 | 2.51 | 0.45 |
| 5:HC:597:ARG:HH12 | 5:HD:489:GLY:N | 2.14 | 0.45 |
| 5:HD:137:TYR:HD1 | 5:HD:143:TRP:HE1 | 1.61 | 0.45 |
| 5:HD:304:ILE:HD11 | 5:HD:366:PRO:HG3 | 1.99 | 0.45 |
| 6:HF:126:VAL:HG12 | 6:HF:130:ARG:NH1 | 2.31 | 0.45 |
| 6:HG:126:VAL:HG12 | 6:HG:130:ARG:NH1 | 2.31 | 0.45 |
| 7:HH:132:ARG:O | 7:HH:141:VAL:HG12 | 2.17 | 0.45 |
| 7:HI:162:PRO:O | 7:HI:165:THR:N | 2.49 | 0.45 |
| 7:HI:227:VAL:HG23 | 7:HJ:225:LYS:HB3 | 1.99 | 0.45 |
| 7:HJ:100:TYR:CE1 | 7:HJ:115:SER:HB2 | 2.52 | 0.45 |
| 5:I:361:ASP:N | 5:I:365:ILE:O | 2.50 | 0.45 |
| 8:IA:70:THR:HG22 | 8:IA:156:THR:HG22 | 1.98 | 0.45 |
| 8:IA:40:ALA:O | 8:IA:69:TRP:NE1 | 2.49 | 0.45 |
| 8:IB:15:PHE:N | 8:IB:15:PHE:CD1 | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:IB:70:THR:HG22 | 8:IB:156:THR:HG22 | 1.98 | 0.45 |
| 9:IC:96:ILE:O | 9:IC:105:ILE:HG22 | 2.17 | 0.45 |
| 12:GC:153:ARG:HH22 | 12:IF:184:PRO:HA | 1.81 | 0.45 |
| 12:IF:21:MET:HB3 | 12:IF:204:HIS:O | 2.15 | 0.45 |
| 12:GC:16:PHE:CB | 12:IF:236:ILE:HD11 | 2.46 | 0.45 |
| 5:J:186:TYR:HB3 | 5:J:227:GLY:CA | 2.46 | 0.45 |
| 5:J:359:GLU:H | 5:J:370:HIS:C | 2.16 | 0.45 |
| 5:K:137:TYR:HA | 5:K:143:TRP:HD1 | 1.81 | 0.45 |
| 5:K:22:GLY:O | 5:K:26:ILE:HG22 | 2.16 | 0.45 |
| 6:L:19:GLY:N | 6:M:13:ARG:NH1 | 2.64 | 0.45 |
| 6:M:100:PRO:O | 6:M:103:SER:OG | 2.18 | 0.45 |
| 7:P:162:PRO:O | 7:P:165:THR:N | 2.49 | 0.45 |
| 7:P:173:ILE:HD12 | 7:P:176:ILE:HG21 | 1.99 | 0.45 |
| 7:P:348:MET:SD | 7:Q:400:VAL:HG11 | 2.56 | 0.45 |
| 7:O:60:ILE:HG22 | 7:P:52:SER:N | 2.31 | 0.45 |
| 7:Q:415:ASN:O | 7:Q:424:ARG:HD2 | 2.16 | 0.45 |
| 9:T:72:THR:OG1 | 10:U:126:ASN:ND2 | 2.43 | 0.45 |
| 10:U:312:GLY:HA2 | 10:U:313:PRO:HA | 1.80 | 0.45 |
| 10:U:207:PHE:O | 10:U:345:GLU:HA | 2.16 | 0.45 |
| 1:X:227:ARG:HB2 | 1:X:237:TYR:CE2 | 2.51 | 0.45 |
| 1:X:200:TYR:HB2 | 1:X:269:VAL:HG13 | 1.98 | 0.45 |
| 1:Y:348:PHE:HZ | 1:Y:399:TYR:CD2 | 2.34 | 0.45 |
| 1:Y:472:ASP:OD2 | 1:Y:474:SER:HB2 | 2.17 | 0.45 |
| 1:Y:73:ALA:O | 1:Y:77:GLU:HB2 | 2.16 | 0.45 |
| 13:YA:315[C]:LEU:O | 13:YA:319[C]:GLN:HG2 | 2.16 | 0.45 |
| 13:YA:407[C]:PRO:HB3 | 13:YC:232[C]:ASN:CB | 2.47 | 0.45 |
| 13:YA:407[F]:PRO:HB3 | 13:YC:232[F]:ASN:CB | 2.47 | 0.45 |
| 13:YA:470[A]:ARG:HD2 | 13:YC:474[A]:ILE:HD11 | 1.97 | 0.45 |
| 13:YA:478[A]:ASN:N | 13:YC:485[A]:ASP:O | 2.49 | 0.45 |
| 13:YA:554[D]:MET:HA | 13:YB:546[D]:VAL:O | 2.17 | 0.45 |
| 13:YA:554[E]:MET:HA | 13:YB:546[E]:VAL:O | 2.16 | 0.45 |
| 13:YA:76[B]:PRO:HB2 | 13:YA:98[B]:GLY:C | 2.37 | 0.45 |
| 13:YB:148[C]:GLN:NE2 | 13:YB:421[C]:TYR:OH | 2.49 | 0.45 |
| 13:YB:252[E]:MET:HB3 | 13:YB:252[E]:MET:HE3 | 1.74 | 0.45 |
| 13:YB:266[C]:TRP:CD1 | 13:YB:274[C]:GLN:HG2 | 2.51 | 0.45 |
| 13:YB:315[B]:LEU:O | 13:YB:319[B]:GLN:HG2 | 2.16 | 0.45 |
| 13:YA:315[C]:LEU:HD23 | 13:YB:367[C]:PRO:HA | 1.97 | 0.45 |
| 13:YB:481[B]:PHE:O | 13:YC:473[B]:GLN:HA | 2.15 | 0.45 |
| 13:YA:554[B]:MET:HA | 13:YB:546[B]:VAL:O | 2.16 | 0.45 |
| 13:YA:558[E]:SER:O | 13:YB:551[E]:THR:HA | 2.16 | 0.45 |
| 13:YB:551[D]:THR:O | 13:YC:543[D]:ASP:HA | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:568[D]:ASP:OD1 | 13:YB:569[D]:GLY:N | 2.49 | 0.45 |
| 13:YC:121[A]:TYR:OH | 13:YC:123[A]:ARG:NH2 | 2.50 | 0.45 |
| 13:YC:121[F]:TYR:OH | 13:YC:123[F]:ARG:NH2 | 2.49 | 0.45 |
| 13:YC:146[E]:VAL:O | 13:YC:150[E]:SER:OG | 2.34 | 0.45 |
| 13:YC:252[A]:MET:HB3 | 13:YC:252[A]:MET:HE3 | 1.83 | 0.45 |
| 13:YC:266[F]:TRP:CD1 | 13:YC:274[F]:GLN:HG2 | 2.51 | 0.45 |
| 13:YB:315[A]:LEU:HD23 | 13:YC:367[A]:PRO:HA | 1.97 | 0.45 |
| 13:YB:70[D]:GLY:O | 13:YC:394[D]:GLU:N | 2.50 | 0.45 |
| 13:YC:537[F]:LYS:HD3 | 13:YC:537[F]:LYS:C | 2.37 | 0.45 |
| 13:YB:551[C]:THR:O | 13:YC:543[C]:ASP:HA | 2.16 | 0.45 |
| 13:YB:561[F]:SER:HA | 13:YC:554[F]:MET:O | 2.16 | 0.45 |
| 14:YD:10[A]:PRO:HD2 | 14:YD:349[A]:ASN:O | 2.16 | 0.45 |
| 14:YD:127[C]:ASP:CG | 14:YD:130[C]:GLU:H | 2.20 | 0.45 |
| 14:YD:135[C]:MET:SD | 14:YD:166[C]:PHE:HD1 | 2.40 | 0.45 |
| 14:YD:266[F]:ILE:HD11 | 14:YD:290[F]:ASN:CG | 2.36 | 0.45 |
| 14:YD:307[C]:TYR:HD1 | 14:YD:307[C]:TYR:HA | 1.66 | 0.45 |
| 14:YD:61[E]:HIS:NE2 | 14:YF:332[E]:GLN:HB3 | 2.31 | 0.45 |
| 14:YD:20[C]:TYR:HA | 14:YD:69[C]:ILE:HD12 | 1.98 | 0.45 |
| 14:YE:212[A]:ILE:HG22 | 14:YE:327[A]:ASN:HB2 | 1.98 | 0.45 |
| 14:YE:73[C]:SER:HB2 | 14:YE:85[C]:THR:HG23 | 1.99 | 0.45 |
| 14:YF:127[E]:ASP:CG | 14:YF:130[E]:GLU:H | 2.20 | 0.45 |
| 11:BF:175:SER:HA | 14:YF:217[E]:SER:HB2 | 1.97 | 0.45 |
| 14:YF:266[F]:ILE:HD11 | 14:YF:290[F]:ASN:CG | 2.36 | 0.45 |
| 14:YF:236[C]:TRP:CD1 | 14:YF:308[C]:ALA:HB2 | 2.51 | 0.45 |
| 14:YF:20[D]:TYR:HA | 14:YF:69[D]:ILE:HD12 | 1.99 | 0.45 |
| 2:Z:369:ASP:HB2 | 2:Z:434:MET:HG2 | 1.99 | 0.45 |
| 2:Z:975:ASN:OD1 | 2:Z:981:GLN:HB3 | 2.16 | 0.45 |
| 1:A:328:LEU:HA | 1:A:328:LEU:HD23 | 1.71 | 0.45 |
| 1:A:339:CYS:SG | 1:A:400:ASN:HA | 2.57 | 0.45 |
| 1:A:440:ILE:HG13 | 1:A:441:ILE:N | 2.31 | 0.45 |
| 5:AC:214:SER:HB2 | 5:AC:225:LEU:HA | 1.99 | 0.45 |
| 5:AC:361:ASP:N | 5:AC:365:ILE:O | 2.50 | 0.45 |
| 5:AC:85:THR:HB | 5:AC:137:TYR:CE2 | 2.52 | 0.45 |
| 5:AD:107:VAL:O | 5:AD:125:GLU:HG3 | 2.16 | 0.45 |
| 5:AD:503:ASN:OD1 | 5:AD:504:ASN:N | 2.49 | 0.45 |
| 6:AF:107:VAL:HG22 | 6:AF:174:TYR:HD2 | 1.82 | 0.45 |
| 6:AF:126:VAL:HG12 | 6:AF:130:ARG:NH1 | 2.31 | 0.45 |
| 7:AI:415:ASN:O | 7:AI:424:ARG:HD2 | 2.17 | 0.45 |
| 7:AJ:165:THR:HA | 7:AJ:168:LEU:HB2 | 1.98 | 0.45 |
| 7:AJ:77:THR:HA | 7:BA:74:LYS:O | 2.17 | 0.45 |
| 1:B:647:ARG:HD3 | 1:B:650:TYR:CE2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:BB:22:GLN:HE21 | 8:BB:33:THR:HG21 | 1.81 | 0.45 |
| 8:BC:112:ILE:HD11 | 8:BC:126:GLU:OE2 | 2.15 | 0.45 |
| 8:R:2:PHE:CD2 | 8:BC:98:GLU:HA | 2.51 | 0.45 |
| 1:BI:346:ASP:O | 1:BI:350:SER:N | 2.50 | 0.45 |
| 1:BI:374:ILE:HB | 1:BI:408:ILE:HG12 | 1.98 | 0.45 |
| 1:BI:583:SER:OG | 1:BI:584:ASP:N | 2.49 | 0.45 |
| 2:BJ:120:ASN:CB | 2:BJ:155:PRO:HB3 | 2.35 | 0.45 |
| 2:BJ:347:GLU:CG | 2:BJ:349:LEU:HD21 | 2.46 | 0.45 |
| 2:C:525:TRP:CE2 | 2:C:526:ILE:O | 2.68 | 0.45 |
| 2:C:604:VAL:HG22 | 2:C:605:ARG:H | 1.80 | 0.45 |
| 2:C:675:LEU:HD12 | 2:C:675:LEU:HA | 1.67 | 0.45 |
| 3:CB:17:ARG:HD2 | 3:CB:334:PHE:OXT | 2.17 | 0.45 |
| 3:CB:95:TRP:CH2 | 3:CB:169:PRO:HD3 | 2.51 | 0.45 |
| 4:CE:22:ASP:O | 4:CE:26:ASP:N | 2.26 | 0.45 |
| 5:CF:214:SER:HB2 | 5:CF:215:PRO:HD2 | 1.98 | 0.45 |
| 5:CF:268:SER:N | 5:CF:283:THR:O | 2.35 | 0.45 |
| 5:CF:322:GLY:HA2 | 5:CF:360:THR:H | 1.81 | 0.45 |
| 5:CF:591:PRO:HD3 | 5:CG:522:SER:C | 2.37 | 0.45 |
| 5:CG:190:ASN:HD22 | 5:CG:247:PHE:HD2 | 1.64 | 0.45 |
| 5:CF:49:TRP:C | 5:CH:90:ASN:HD21 | 2.10 | 0.45 |
| 6:CI:13:ARG:HG2 | 6:CI:14:LEU:N | 2.27 | 0.45 |
| 6:CI:71:ILE:O | 6:CI:215:PHE:N | 2.36 | 0.45 |
| 3:D:174:GLY:HA3 | 3:D:180:ILE:HG12 | 1.97 | 0.45 |
| 3:D:257:TYR:HB3 | 3:D:296:TYR:CE2 | 2.50 | 0.45 |
| 3:D:93:ARG:HH21 | 3:D:106:PHE:HD1 | 1.64 | 0.45 |
| 6:DA:12:SER:HG | 6:DA:17:PHE:HD2 | 1.63 | 0.45 |
| 6:DA:203:LEU:HD12 | 6:DA:206:GLN:NE2 | 2.31 | 0.45 |
| 7:DB:146:SER:N | 7:DC:136:GLU:OE1 | 2.50 | 0.45 |
| 7:DB:509:GLY:HA3 | 7:DC:441:GLN:HE21 | 1.82 | 0.45 |
| 7:DD:415:ASN:O | 7:DD:424:ARG:HD2 | 2.16 | 0.45 |
| 8:DE:114:ARG:HD2 | 8:DE:123:VAL:HG11 | 1.97 | 0.45 |
| 8:DF:70:THR:HG22 | 8:DF:156:THR:HG22 | 1.98 | 0.45 |
| 3:E:233:GLN:NE2 | 2:GF:528:ASN:HB3 | 2.32 | 0.45 |
| 1:EA:243:ILE:HG22 | 1:EA:258:GLY:CA | 2.45 | 0.45 |
| 1:EA:336:GLN:HG3 | 1:EA:337:GLN:N | 2.32 | 0.45 |
| 1:EA:440:ILE:HD11 | 1:EA:653:ILE:HG21 | 1.98 | 0.45 |
| 1:EA:654:ASP:OD1 | 1:EA:655:LEU:N | 2.49 | 0.45 |
| 1:EB:121:ASN:HA | 1:EB:155:ARG:HD3 | 1.99 | 0.45 |
| 1:EB:346:ASP:O | 1:EB:350:SER:N | 2.50 | 0.45 |
| 1:EB:348:PHE:HZ | 1:EB:399:TYR:CD2 | 2.34 | 0.45 |
| 1:EB:470:ASP:O | 1:EB:472:ASP:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:647:ARG:HD3 | 1:EB:650:TYR:CE2 | 2.50 | 0.45 |
| 2:EC:425:ARG:NH2 | 2:EC:447:ASN:HD21 | 2.14 | 0.45 |
| 2:EC:516:TRP:HE1 | 2:EC:518:LYS:CG | 2.29 | 0.45 |
| 2:EC:645:LEU:HD11 | 11:GB:83:TYR:CD1 | 2.51 | 0.45 |
| 2:EC:651:THR:HG21 | 11:GB:55:ARG:HD3 | 1.98 | 0.45 |
| 2:EC:694:TYR:HD2 | 2:EC:696:ARG:N | 2.05 | 0.45 |
| 2:EC:761:GLU:HB2 | 2:EC:862:TYR:CZ | 2.51 | 0.45 |
| 3:ED:23:ASN:OD1 | 3:EE:27:SER:OG | 2.17 | 0.45 |
| 3:EE:24:PHE:O | 3:EE:28:ILE:HD12 | 2.16 | 0.45 |
| 3:EE:76:MET:O | 3:EE:299:PRO:HD3 | 2.16 | 0.45 |
| 5:EI:85:THR:HB | 5:EI:137:TYR:CE2 | 2.52 | 0.45 |
| 5:EI:554:GLY:O | 5:EI:555:CYS:SG | 2.75 | 0.45 |
| 5:EI:591:PRO:HD3 | 5:EJ:522:SER:C | 2.37 | 0.45 |
| 5:EJ:161:ASN:OD1 | 5:EJ:249:ASP:HB3 | 2.16 | 0.45 |
| 5:EJ:305:ASN:HB3 | 5:FA:255:ARG:HH12 | 1.81 | 0.45 |
| 5:EJ:567:THR:O | 5:FA:551:ILE:HA | 2.16 | 0.45 |
| 5:EJ:97:ASP:OD1 | 5:EJ:102:TRP:CE2 | 2.68 | 0.45 |
| 5:FA:151:ILE:HG23 | 5:FA:152:ASP:H | 1.81 | 0.45 |
| 5:FA:265:LEU:HB3 | 5:FA:281:TYR:HB3 | 1.99 | 0.45 |
| 5:FA:372:ASP:N | 5:FA:372:ASP:OD1 | 2.48 | 0.45 |
| 5:FA:267:ASP:CG | 5:FA:377:HIS:HA | 2.37 | 0.45 |
| 5:EJ:357:SER:OG | 6:FB:4:LEU:HD21 | 2.16 | 0.45 |
| 6:FC:144:ASN:HB3 | 6:FC:159:THR:HG22 | 1.99 | 0.45 |
| 6:FC:43:LEU:O | 6:FD:111:GLY:HA3 | 2.16 | 0.45 |
| 7:FE:357:ASP:OD1 | 7:FF:339:ARG:NH2 | 2.49 | 0.45 |
| 7:FE:65:GLU:O | 7:FE:69:GLY:N | 2.48 | 0.45 |
| 7:FE:161:THR:HA | 7:FF:158:THR:O | 2.17 | 0.45 |
| 7:FE:300:LEU:HB3 | 7:FF:302:ILE:HD13 | 1.98 | 0.45 |
| 7:FE:418:ASP:OD2 | 7:FF:505:PRO:HD3 | 2.15 | 0.45 |
| 7:FF:57:ILE:HG23 | 7:FG:56:GLY:CA | 2.46 | 0.45 |
| 7:FE:39:ILE:HA | 7:FG:44:VAL:HG22 | 1.97 | 0.45 |
| 7:FG:87:TYR:CZ | 7:FG:97:LEU:HD12 | 2.51 | 0.45 |
| 8:FH:22:GLN:HE21 | 8:FH:33:THR:HG21 | 1.81 | 0.45 |
| 8:FI:41:LEU:HD22 | 8:IB:140:LEU:HD23 | 1.98 | 0.45 |
| 4:G:111:ASN:HB2 | 4:G:116:ILE:HD12 | 1.98 | 0.45 |
| 4:G:79:VAL:N | 4:G:97:ILE:O | 2.32 | 0.45 |
| 11:GB:14:LYS:O | 11:GB:15:THR:HG22 | 2.17 | 0.45 |
| 1:GD:619:GLN:CD | 1:GD:619:GLN:H | 2.18 | 0.45 |
| 1:GE:538:VAL:HG11 | 1:GE:558:PHE:HE1 | 1.80 | 0.45 |
| 1:GE:647:ARG:HD3 | 1:GE:650:TYR:CE2 | 2.50 | 0.45 |
| 2:GF:425:ARG:NH2 | 2:GF:447:ASN:HD21 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:825:GLU:HA | 2:GF:836:GLY:O | 2.16 | 0.45 |
| 3:GG:68:VAL:O | 3:GG:71:MET:HB3 | 2.16 | 0.45 |
| 4:GI:1:MET:HG2 | 4:GI:70:HIS:ND1 | 2.32 | 0.45 |
| 5:HB:196:ARG:HD3 | 7:HH:5:THR:HG23 | 1.97 | 0.45 |
| 5:HB:214:SER:HB2 | 5:HB:225:LEU:HA | 1.99 | 0.45 |
| 5:HB:322:GLY:HA2 | 5:HB:360:THR:H | 1.81 | 0.45 |
| 5:HB:554:GLY:O | 5:HB:555:CYS:SG | 2.75 | 0.45 |
| 5:HC:247:PHE:CZ | 5:HD:162:VAL:HG11 | 2.51 | 0.45 |
| 5:HC:363:ASN:N | 5:HC:367:GLU:OE2 | 2.49 | 0.45 |
| 5:HC:260:ARG:HA | 5:HC:384:THR:HA | 1.98 | 0.45 |
| 5:HC:304:ILE:CD1 | 5:HC:385:TRP:HA | 2.40 | 0.45 |
| 5:HD:356:TYR:HE1 | 6:HF:4:LEU:HD13 | 1.81 | 0.45 |
| 7:HH:401:ARG:NH2 | 7:HJ:397:GLY:O | 2.49 | 0.45 |
| 7:HJ:63:GLU:O | 7:HJ:67:ILE:HG12 | 2.16 | 0.45 |
| 7:HJ:88:PRO:HG2 | 7:HJ:95:TYR:O | 2.16 | 0.45 |
| 5:I:214:SER:HB2 | 5:I:225:LEU:HA | 1.99 | 0.45 |
| 5:I:290:SER:N | 5:I:371:PHE:O | 2.49 | 0.45 |
| 1:GD:52:ARG:HH21 | 9:IC:25:ARG:HB3 | 1.81 | 0.45 |
| 5:J:322:GLY:HA2 | 5:J:360:THR:H | 1.81 | 0.45 |
| 5:J:503:ASN:OD1 | 5:J:504:ASN:N | 2.49 | 0.45 |
| 5:I:591:PRO:HD3 | 5:J:522:SER:C | 2.37 | 0.45 |
| 5:I:164:ARG:NH1 | 5:K:192:ARG:HD3 | 2.32 | 0.45 |
| 6:N:203:LEU:HD12 | 6:N:206:GLN:NE2 | 2.31 | 0.45 |
| 7:P:59:PHE:CZ | 7:Q:55:LYS:HG3 | 2.52 | 0.45 |
| 7:Q:418:ASP:OD2 | 7:Q:422:LYS:HB2 | 2.16 | 0.45 |
| 10:U:323:LYS:O | 10:U:324:THR:OG1 | 2.33 | 0.45 |
| 10:U:57:LEU:HG | 12:IF:144:ASN:ND2 | 2.32 | 0.45 |
| 12:W:24:CYS:CB | 12:W:125:ILE:HD13 | 2.46 | 0.45 |
| 1:X:106:ALA:HB3 | 1:X:169:GLN:HB2 | 1.98 | 0.45 |
| 1:X:568:ASN:OD1 | 1:X:569:ILE:N | 2.50 | 0.45 |
| 13:YA:110[A]:ARG:HD2 | 13:YA:118[A]:THR:O | 2.17 | 0.45 |
| 13:YA:121[D]:TYR:HB3 | 13:YC:66[D]:MET:SD | 2.55 | 0.45 |
| 13:YA:146[C]:VAL:O | 13:YA:150[C]:SER:OG | 2.34 | 0.45 |
| 13:YA:146[D]:VAL:O | 13:YA:150[D]:SER:OG | 2.34 | 0.45 |
| 13:YA:146[F]:VAL:O | 13:YA:150[F]:SER:OG | 2.34 | 0.45 |
| 13:YA:18[B]:ARG:CZ | 13:YA:77[B]:VAL:HG23 | 2.46 | 0.45 |
| 13:YA:543[E]:ASP:HA | 13:YC:551[E]:THR:O | 2.17 | 0.45 |
| 13:YA:543[F]:ASP:HA | 13:YC:551[F]:THR:O | 2.17 | 0.45 |
| 13:YA:571[A]:ARG:HD3 | 13:YB:564[A]:GLN:HE22 | 1.82 | 0.45 |
| 13:YA:574[C]:ILE:O | 15:ZA:70[C]:THR:N | 2.27 | 0.45 |
| 13:YA:60[F]:PRO:HB3 | 13:YB:60[F]:PRO:HB3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:61[B]:ILE:HB | 13:YB:75[B]:GLY:HA2 | 1.98 | 0.45 |
| 13:YA:71[D]:GLY:HA2 | 13:YB:393[D]:MET:HA | 1.97 | 0.45 |
| 13:YA:76[F]:PRO:O | 13:YC:61[F]:ILE:HA | 2.17 | 0.45 |
| 13:YB:266[A]:TRP:CD1 | 13:YB:274[A]:GLN:HG2 | 2.52 | 0.45 |
| 13:YB:266[D]:TRP:CD1 | 13:YB:274[D]:GLN:HG2 | 2.52 | 0.45 |
| 13:YB:315[A]:LEU:O | 13:YB:319[A]:GLN:HG2 | 2.16 | 0.45 |
| 13:YB:416[E]:HIS:CG | 13:YB:417[E]:PRO:HD2 | 2.51 | 0.45 |
| 13:YA:498[C]:VAL:HA | 13:YB:490[C]:VAL:O | 2.16 | 0.45 |
| 13:YB:537[B]:LYS:HD3 | 13:YB:537[B]:LYS:C | 2.37 | 0.45 |
| 13:YB:69[B]:ILE:HG12 | 13:YC:396[B]:GLU:HA | 1.97 | 0.45 |
| 13:YB:18[B]:ARG:CZ | 13:YB:77[B]:VAL:HG23 | 2.46 | 0.45 |
| 13:YB:73[F]:VAL:HG21 | 13:YC:129[F]:THR:HG22 | 1.99 | 0.45 |
| 13:YC:146[A]:VAL:O | 13:YC:150[A]:SER:OG | 2.34 | 0.45 |
| 13:YC:315[F]:LEU:O | 13:YC:319[F]:GLN:HG2 | 2.16 | 0.45 |
| 13:YB:71[D]:GLY:HA2 | 13:YC:393[D]:MET:HA | 1.98 | 0.45 |
| 13:YC:490[A]:VAL:HG12 | 13:YC:492[A]:GLY:H | 1.82 | 0.45 |
| 13:YA:534[F]:LEU:CB | 13:YC:538[F]:VAL:HG11 | 2.47 | 0.45 |
| 13:YA:550[C]:TRP:O | 13:YC:558[C]:SER:N | 2.48 | 0.45 |
| 14:YD:117[E]:ASN:O | 14:YD:119[E]:LYS:HG3 | 2.17 | 0.45 |
| 13:YA:47[C]:ILE:HG12 | 14:YD:123[C]:PRO:HD3 | 1.99 | 0.45 |
| 14:YD:135[B]:MET:SD | 14:YD:166[B]:PHE:HD1 | 2.40 | 0.45 |
| 14:YD:140[B]:TYR:CD2 | 14:YD:147[B]:THR:HA | 2.51 | 0.45 |
| 14:YD:170[F]:LEU:HA | 14:YD:170[F]:LEU:HD23 | 1.69 | 0.45 |
| 14:YD:212[B]:ILE:HG22 | 14:YD:327[B]:ASN:HB2 | 1.97 | 0.45 |
| 11:V:178:ASN:HB3 | 14:YD:217[A]:SER:H | 1.82 | 0.45 |
| 11:BF:182:ASN:ND2 | 14:YD:327[C]:ASN:HD22 | 2.15 | 0.45 |
| 14:YD:73[C]:SER:HB2 | 14:YD:85[C]:THR:HG23 | 1.99 | 0.45 |
| 14:YE:117[E]:ASN:O | 14:YE:119[E]:LYS:HG3 | 2.17 | 0.45 |
| 14:YE:160[B]:ILE:HG21 | 14:YE:282[B]:ALA:HB1 | 1.97 | 0.45 |
| 14:YE:160[E]:ILE:HG21 | 14:YE:282[E]:ALA:HB1 | 1.97 | 0.45 |
| 14:YE:135[F]:MET:SD | 14:YE:166[F]:PHE:HD1 | 2.40 | 0.45 |
| 14:YE:266[A]:ILE:HD11 | 14:YE:290[A]:ASN:CG | 2.36 | 0.45 |
| 14:YE:266[B]:ILE:HD11 | 14:YE:290[B]:ASN:CG | 2.36 | 0.45 |
| 14:YE:336[F]:GLU:O | 14:YE:359[F]:THR:OG1 | 2.33 | 0.45 |
| 14:YD:234[C]:PHE:HD1 | 14:YE:97[C]:VAL:HG12 | 1.82 | 0.45 |
| 14:YF:127[A]:ASP:CG | 14:YF:130[A]:GLU:H | 2.20 | 0.45 |
| 14:YF:135[E]:MET:SD | 14:YF:166[E]:PHE:HD1 | 2.40 | 0.45 |
| 14:YF:277[D]:VAL:HG11 | 14:YF:294[D]:GLU:HG2 | 1.98 | 0.45 |
| 14:YF:307[E]:TYR:HA | 14:YF:307[E]:TYR:HD1 | 1.66 | 0.45 |
| 14:YF:236[D]:TRP:CD1 | 14:YF:308[D]:ALA:HB2 | 2.51 | 0.45 |
| 14:YF:288[A]:TYR:CE1 | 14:YF:371[A]:LYS:HD3 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:73[A]:SER:HB2 | 14:YF:85[A]:THR:HG23 | 1.99 | 0.45 |
| 2:Z:202:PHE:HB3 | 2:Z:209:VAL:HG22 | 1.99 | 0.45 |
| 2:Z:549:PRO:HB2 | 2:Z:550:GLU:OE1 | 2.17 | 0.45 |
| 2:Z:708:ILE:HG13 | 2:Z:727:PHE:CE2 | 2.51 | 0.45 |
| 15:ZA:66[C]:LYS:O | 15:ZA:68[C]:TYR:HD1 | 1.99 | 0.45 |
| 5:AD:304:ILE:CD1 | 5:AD:385:TRP:HA | 2.40 | 0.45 |
| 5:AE:192:ARG:HB2 | 5:AE:245:GLU:HB2 | 1.99 | 0.45 |
| 5:AE:267:ASP:H | 5:AE:377:HIS:HB2 | 1.80 | 0.45 |
| 5:AE:310:GLU:HB2 | 5:AE:384:THR:CB | 2.47 | 0.45 |
| 6:AG:126:VAL:HG12 | 6:AG:130:ARG:NH1 | 2.31 | 0.45 |
| 7:AI:263:VAL:O | 7:AJ:255:SER:OG | 2.15 | 0.45 |
| 7:AI:288:ILE:O | 7:AJ:288:ILE:N | 2.43 | 0.45 |
| 7:AJ:228:ILE:HG21 | 7:AJ:244:ALA:HB2 | 1.97 | 0.45 |
| 1:B:197:VAL:HG11 | 1:B:236:PHE:CZ | 2.52 | 0.45 |
| 7:BA:100:TYR:CE1 | 7:BA:115:SER:HB2 | 2.52 | 0.45 |
| 7:BA:118:PRO:O | 7:BA:122:THR:N | 2.41 | 0.45 |
| 1:BI:206:TRP:CE2 | 1:BI:222:THR:HB | 2.52 | 0.45 |
| 1:BI:470:ASP:O | 1:BI:472:ASP:N | 2.50 | 0.45 |
| 1:BI:634:THR:HB | 1:BI:638:SER:O | 2.17 | 0.45 |
| 2:BJ:319:TYR:HD1 | 2:BJ:328:TYR:CB | 2.29 | 0.45 |
| 2:BJ:573:VAL:O | 2:BJ:609:GLU:HA | 2.15 | 0.45 |
| 2:C:314:THR:HB | 2:C:375:VAL:HG11 | 1.98 | 0.45 |
| 2:C:425:ARG:NH2 | 2:C:447:ASN:HD21 | 2.14 | 0.45 |
| 2:C:761:GLU:HB2 | 2:C:862:TYR:CZ | 2.51 | 0.45 |
| 2:C:81:ARG:HD3 | 2:C:96:TYR:CE1 | 2.51 | 0.45 |
| 2:C:912:ILE:HD11 | 3:D:329:ASN:HD22 | 1.81 | 0.45 |
| 5:CF:318:GLN:NE2 | 6:DA:7:LYS:HB3 | 2.32 | 0.45 |
| 5:CF:402:GLU:HG3 | 5:CF:406:LEU:CD1 | 2.47 | 0.45 |
| 5:CG:186:TYR:HB3 | 5:CG:227:GLY:CA | 2.46 | 0.45 |
| 5:CH:132:ASP:OD2 | 5:CH:151:ILE:HA | 2.16 | 0.45 |
| 5:CF:164:ARG:NH1 | 5:CH:192:ARG:HD3 | 2.32 | 0.45 |
| 5:CH:304:ILE:HD11 | 5:CH:366:PRO:HG3 | 1.99 | 0.45 |
| 5:CH:310:GLU:HB2 | 5:CH:384:THR:CB | 2.47 | 0.45 |
| 3:D:294:LYS:N | 3:D:297:TYR:OH | 2.42 | 0.45 |
| 3:D:249:PHE:O | 3:D:329:ASN:HA | 2.16 | 0.45 |
| 7:DB:231:GLY:H | 7:DB:243:VAL:HB | 1.82 | 0.45 |
| 7:DC:418:ASP:HA | 7:DC:424:ARG:NH2 | 2.32 | 0.45 |
| 7:DB:97:LEU:HD22 | 7:DC:96:GLY:HA2 | 1.98 | 0.45 |
| 7:DB:463:THR:HG23 | 7:DD:483:PHE:HE1 | 1.80 | 0.45 |
| 7:DD:77:THR:HG22 | 7:DD:80:THR:H | 1.82 | 0.45 |
| 8:DE:69:TRP:CZ3 | 8:DE:157:LEU:HD12 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:DI:186:ARG:HG2 | 11:DI:187:ILE:H | 1.82 | 0.45 |
| 12:DJ:122:GLY:O | 12:DJ:125:ILE:HG22 | 2.17 | 0.45 |
| 3:E:95:TRP:CH2 | 3:E:169:PRO:HD3 | 2.51 | 0.45 |
| 1:EA:229:THR:OG1 | 1:EA:233:ASN:O | 2.35 | 0.45 |
| 1:EA:619:GLN:CD | 1:EA:619:GLN:H | 2.18 | 0.45 |
| 1:EB:472:ASP:OD2 | 1:EB:474:SER:HB2 | 2.17 | 0.45 |
| 2:EC:726:PHE:O | 2:EC:729:SER:OG | 2.16 | 0.45 |
| 2:EC:708:ILE:HG13 | 2:EC:727:PHE:CE2 | 2.51 | 0.45 |
| 2:EC:802:TYR:CE1 | 2:EC:807:LEU:HB3 | 2.51 | 0.45 |
| 2:EC:81:ARG:HD3 | 2:EC:96:TYR:CE1 | 2.51 | 0.45 |
| 2:EC:965:LEU:HG | 2:EC:982:LEU:HD11 | 1.98 | 0.45 |
| 4:EG:201:LYS:NZ | 4:EG:220:ASN:OD1 | 2.37 | 0.45 |
| 5:EI:204:ASP:OD1 | 5:EI:205:VAL:N | 2.50 | 0.45 |
| 5:EI:312:ARG:HG2 | 5:EI:317:LEU:CA | 2.44 | 0.45 |
| 5:EJ:326:MET:HE3 | 5:EJ:326:MET:HB2 | 1.70 | 0.45 |
| 5:EJ:569:TYR:HD1 | 5:FA:544:VAL:HA | 1.81 | 0.45 |
| 5:FA:358:VAL:HG22 | 5:FA:371:PHE:HB2 | 1.98 | 0.45 |
| 6:FB:126:VAL:HG12 | 6:FB:130:ARG:NH1 | 2.31 | 0.45 |
| 6:FC:126:VAL:HG12 | 6:FC:130:ARG:NH1 | 2.31 | 0.45 |
| 7:FF:360:ARG:HH11 | 7:FF:525:VAL:HG21 | 1.80 | 0.45 |
| 8:FH:79:HIS:HE1 | 8:FH:151:GLN:HE22 | 1.63 | 0.45 |
| 8:FI:135:THR:HG22 | 8:FI:156:THR:O | 2.16 | 0.45 |
| 8:FI:15:PHE:N | 8:FI:15:PHE:CD1 | 2.84 | 0.45 |
| 8:FI:32:PHE:O | 8:FI:35:GLN:N | 2.50 | 0.45 |
| 8:FI:46:VAL:HG13 | 8:FI:63:ASP:O | 2.16 | 0.45 |
| 9:DG:114:ASP:O | 11:GB:47:THR:OG1 | 2.33 | 0.45 |
| 1:GD:440:ILE:HG13 | 1:GD:441:ILE:N | 2.31 | 0.45 |
| 1:GE:200:TYR:HB2 | 1:GE:269:VAL:HG13 | 1.97 | 0.45 |
| 1:GE:374:ILE:HB | 1:GE:408:ILE:HG12 | 1.99 | 0.45 |
| 1:GE:451:ASP:O | 1:GE:454:ILE:HD12 | 2.17 | 0.45 |
| 2:GF:209:VAL:O | 2:GF:221:ALA:HA | 2.16 | 0.45 |
| 2:GF:604:VAL:HG22 | 2:GF:605:ARG:H | 1.80 | 0.45 |
| 2:GF:706:SER:O | 2:GF:708:ILE:N | 2.42 | 0.45 |
| 2:GF:802:TYR:CE1 | 2:GF:807:LEU:HB3 | 2.51 | 0.45 |
| 3:GH:17:ARG:HD2 | 3:GH:334:PHE:OXT | 2.17 | 0.45 |
| 3:GH:197:ASP:OD1 | 3:GH:198:VAL:N | 2.48 | 0.45 |
| 5:HB:258:TYR:CD2 | 5:HD:386:PHE:HE2 | 2.34 | 0.45 |
| 5:HC:147:LYS:O | 5:HC:147:LYS:HG3 | 2.16 | 0.45 |
| 5:HD:151:ILE:HG23 | 5:HD:152:ASP:H | 1.81 | 0.45 |
| 5:HD:358:VAL:HG22 | 5:HD:371:PHE:HB2 | 1.98 | 0.45 |
| 6:HF:144:ASN:HB3 | 6:HF:159:THR:HG22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:87:TYR:HA | 7:HH:412:PRO:CG | 2.46 | 0.45 |
| 5:I:548:GLY:O | 5:K:568:LYS:HB3 | 2.16 | 0.45 |
| 5:J:34:TYR:O | 5:J:38:GLY:N | 2.37 | 0.45 |
| 5:J:469:PRO:HA | 5:J:472:TYR:CE2 | 2.51 | 0.45 |
| 5:K:563:GLY:N | 5:K:564:PRO:HD3 | 2.31 | 0.45 |
| 6:N:135:GLU:O | 6:N:139:SER:N | 2.26 | 0.45 |
| 7:O:447:HIS:CD2 | 7:Q:447:HIS:CD2 | 3.04 | 0.45 |
| 7:P:165:THR:HA | 7:P:168:LEU:HB2 | 1.98 | 0.45 |
| 8:S:40:ALA:O | 8:S:69:TRP:NE1 | 2.49 | 0.45 |
| 11:V:36:PHE:HZ | 11:V:76:CYS:SG | 2.40 | 0.45 |
| 1:X:347:THR:O | 1:X:351:GLU:N | 2.43 | 0.45 |
| 13:YA:148[C]:GLN:NE2 | 13:YA:421[C]:TYR:OH | 2.49 | 0.45 |
| 13:YA:266[A]:TRP:CD1 | 13:YA:274[A]:GLN:HG2 | 2.52 | 0.45 |
| 13:YA:261[C]:LYS:HE2 | 13:YA:293[C]:ASN:HB3 | 1.99 | 0.45 |
| 13:YA:407[D]:PRO:HB3 | 13:YC:232[D]:ASN:CB | 2.46 | 0.45 |
| 13:YA:478[C]:ASN:N | 13:YC:485[C]:ASP:O | 2.49 | 0.45 |
| 13:YA:537[D]:LYS:C | 13:YA:537[D]:LYS:HD3 | 2.37 | 0.45 |
| 13:YA:554[C]:MET:HA | 13:YB:546[C]:VAL:O | 2.16 | 0.45 |
| 13:YB:109[A]:ASN:OD1 | 13:YB:111[A]:LEU:N | 2.49 | 0.45 |
| 13:YB:109[D]:ASN:OD1 | 13:YB:111[D]:LEU:N | 2.50 | 0.45 |
| 13:YB:121[A]:TYR:OH | 13:YB:123[A]:ARG:NH2 | 2.50 | 0.45 |
| 13:YB:121[D]:TYR:OH | 13:YB:123[D]:ARG:NH2 | 2.50 | 0.45 |
| 13:YB:24[C]:LEU:HD21 | 13:YC:102[C]:GLY:HA2 | 1.99 | 0.45 |
| 13:YB:261[F]:LYS:HE2 | 13:YB:293[F]:ASN:HB3 | 1.99 | 0.45 |
| 13:YB:490[F]:VAL:HG12 | 13:YB:492[F]:GLY:H | 1.81 | 0.45 |
| 13:YB:537[C]:LYS:HD3 | 13:YB:537[C]:LYS:C | 2.37 | 0.45 |
| 13:YB:61[C]:ILE:HG13 | 13:YB:62[C]:THR:N | 2.27 | 0.45 |
| 13:YB:66[C]:MET:HE2 | 13:YC:122[C]:PRO:HB3 | 1.97 | 0.45 |
| 13:YB:7[B]:ASN:OD1 | 13:YC:9[B]:ASN:ND2 | 2.49 | 0.45 |
| 13:YB:76[C]:PRO:HG3 | 13:YB:96[C]:VAL:CG1 | 2.46 | 0.45 |
| 13:YC:110[C]:ARG:HD2 | 13:YC:118[C]:THR:O | 2.17 | 0.45 |
| 13:YC:121[C]:TYR:OH | 13:YC:123[C]:ARG:NH2 | 2.49 | 0.45 |
| 13:YB:73[A]:VAL:HG21 | 13:YC:129[A]:THR:HG22 | 1.99 | 0.45 |
| 13:YC:146[B]:VAL:O | 13:YC:150[B]:SER:OG | 2.34 | 0.45 |
| 13:YC:180[C]:LEU:HD13 | 13:YC:180[C]:LEU:HA | 1.76 | 0.45 |
| 13:YC:266[D]:TRP:CD1 | 13:YC:274[D]:GLN:HG2 | 2.52 | 0.45 |
| 13:YC:315[E]:LEU:O | 13:YC:319[E]:GLN:HG2 | 2.16 | 0.45 |
| 13:YB:481[A]:PHE:O | 13:YC:473[A]:GLN:HA | 2.15 | 0.45 |
| 13:YC:76[C]:PRO:HG3 | 13:YC:96[C]:VAL:CG1 | 2.46 | 0.45 |
| 13:YB:7[E]:ASN:OD1 | 13:YC:9[E]:ASN:ND2 | 2.49 | 0.45 |
| 14:YD:160[C]:ILE:HG21 | 14:YD:282[C]:ALA:HB1 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:178[F]:LEU:CD1 | 14:YD:183[F]:ASP:HA | 2.45 | 0.45 |
| 14:YD:266[C]:ILE:HD11 | 14:YD:290[C]:ASN:CG | 2.37 | 0.45 |
| 14:YD:288[A]:TYR:CE1 | 14:YD:371[A]:LYS:HD3 | 2.52 | 0.45 |
| 14:YD:20[D]:TYR:HA | 14:YD:69[D]:ILE:HD12 | 1.99 | 0.45 |
| 14:YE:140[F]:TYR:CD2 | 14:YE:147[F]:THR:HA | 2.50 | 0.45 |
| 14:YE:178[D]:LEU:CD1 | 14:YE:183[D]:ASP:HA | 2.45 | 0.45 |
| 14:YE:20[C]:TYR:HA | 14:YE:69[C]:ILE:HD12 | 1.98 | 0.45 |
| 14:YE:234[D]:PHE:HD1 | 14:YF:97[D]:VAL:HG12 | 1.82 | 0.45 |
| 14:YE:236[D]:TRP:N | 14:YF:95[D]:VAL:O | 2.50 | 0.45 |
| 14:YE:242[E]:PRO:HD2 | 14:YF:91[E]:LYS:O | 2.16 | 0.45 |
| 14:YE:266[C]:ILE:HD11 | 14:YE:290[C]:ASN:CG | 2.36 | 0.45 |
| 14:YE:10[B]:PRO:HD2 | 14:YE:349[B]:ASN:O | 2.17 | 0.45 |
| 14:YE:20[E]:TYR:HA | 14:YE:69[E]:ILE:HD12 | 1.99 | 0.45 |
| 14:YF:266[A]:ILE:HD11 | 14:YF:290[A]:ASN:CG | 2.36 | 0.45 |
| 14:YF:10[C]:PRO:HD2 | 14:YF:349[C]:ASN:O | 2.16 | 0.45 |
| 1:A:102:SER:OG | 1:A:103:LYS:N | 2.48 | 0.45 |
| 4:AA:1:MET:HG2 | 4:AA:70:HIS:ND1 | 2.32 | 0.45 |
| 5:AC:54:ALA:HB2 | 5:AC:71:ASN:O | 2.16 | 0.45 |
| 5:AC:554:GLY:O | 5:AC:555:CYS:SG | 2.75 | 0.45 |
| 5:AC:584:THR:O | 5:AD:531:ASN:ND2 | 2.44 | 0.45 |
| 5:AC:317:LEU:HD13 | 5:AD:312:ARG:NH1 | 2.32 | 0.45 |
| 5:AD:359:GLU:O | 5:AD:370:HIS:N | 2.45 | 0.45 |
| 5:AD:395:THR:HG22 | 5:AE:307:ASN:HD21 | 1.82 | 0.45 |
| 5:AE:344:VAL:HG12 | 5:AE:349:TRP:H | 1.80 | 0.45 |
| 5:AE:470:VAL:O | 5:AE:474:GLY:N | 2.49 | 0.45 |
| 7:AI:43:GLY:HA3 | 7:AJ:39:ILE:HG23 | 1.98 | 0.45 |
| 1:B:206:TRP:CE2 | 1:B:222:THR:HB | 2.52 | 0.45 |
| 1:B:348:PHE:HZ | 1:B:399:TYR:CD2 | 2.35 | 0.45 |
| 1:B:40:GLN:HE21 | 1:B:43:PHE:HB2 | 1.80 | 0.45 |
| 1:B:451:ASP:O | 1:B:454:ILE:HD12 | 2.17 | 0.45 |
| 7:AJ:45:ASN:CG | 7:BA:24:ASN:HD21 | 2.19 | 0.45 |
| 7:AI:346:ILE:HD11 | 7:BA:350:ALA:HB2 | 1.99 | 0.45 |
| 7:BA:359:TRP:CZ2 | 7:BA:524:LYS:HD3 | 2.52 | 0.45 |
| 7:BA:77:THR:HG22 | 7:BA:80:THR:H | 1.82 | 0.45 |
| 8:BC:70:THR:HG22 | 8:BC:156:THR:HG22 | 1.98 | 0.45 |
| 10:BE:37:GLN:HB3 | 10:BE:128:LEU:HB3 | 1.99 | 0.45 |
| 1:BH:227:ARG:HB2 | 1:BH:237:TYR:HE2 | 1.81 | 0.45 |
| 1:BH:336:GLN:HG3 | 1:BH:337:GLN:N | 2.31 | 0.45 |
| 2:BJ:110:PHE:HB3 | 2:BJ:621:ALA:HA | 1.99 | 0.45 |
| 2:BJ:336:ILE:HG21 | 2:BJ:350:PHE:O | 2.17 | 0.45 |
| 2:BJ:437:ASP:OD1 | 2:BJ:440:LEU:HB2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:81:ARG:HD3 | 2:BJ:96:TYR:CE1 | 2.51 | 0.45 |
| 2:C:244:THR:HB | 2:C:246:TYR:CZ | 2.51 | 0.45 |
| 2:C:338:PHE:CE2 | 2:C:342:SER:O | 2.69 | 0.45 |
| 2:C:347:GLU:CG | 2:C:349:LEU:HD21 | 2.46 | 0.45 |
| 2:C:400:ASP:O | 2:C:424:ARG:NH1 | 2.50 | 0.45 |
| 2:C:982:LEU:HD12 | 2:C:982:LEU:O | 2.17 | 0.45 |
| 3:CA:46:PRO:HA | 3:CA:270:ARG:CZ | 2.47 | 0.45 |
| 5:CF:118:LYS:HZ3 | 5:CF:147:LYS:HD3 | 1.82 | 0.45 |
| 5:CF:135:LEU:HA | 5:CF:144:GLU:O | 2.17 | 0.45 |
| 5:CF:153:LYS:HE3 | 5:CF:155:THR:OG1 | 2.17 | 0.45 |
| 5:CF:334:ALA:HA | 5:CF:349:TRP:NE1 | 2.31 | 0.45 |
| 5:CF:418:GLY:C | 5:CH:472:TYR:HB3 | 2.37 | 0.45 |
| 5:CG:288:MET:HE1 | 5:CG:292:PRO:HD3 | 1.98 | 0.45 |
| 5:CH:157:SER:O | 5:CH:160:SER:OG | 2.28 | 0.45 |
| 5:CH:177:PHE:CD2 | 5:CH:230:ILE:HD11 | 2.48 | 0.45 |
| 5:CH:265:LEU:HB3 | 5:CH:281:TYR:HB3 | 1.99 | 0.45 |
| 5:CH:377:HIS:CG | 5:CH:378:GLY:N | 2.85 | 0.45 |
| 3:D:46:PRO:HA | 3:D:270:ARG:CZ | 2.47 | 0.45 |
| 7:DB:288:ILE:HG13 | 7:DD:288:ILE:HG22 | 1.98 | 0.45 |
| 7:DB:299:THR:O | 7:DD:293:GLY:N | 2.50 | 0.45 |
| 7:DB:448:ALA:HA | 7:DD:483:PHE:HA | 1.99 | 0.45 |
| 5:CF:240:ASP:HA | 7:DB:5:THR:OG1 | 2.16 | 0.45 |
| 7:DC:172:LEU:O | 7:DC:175:GLN:NE2 | 2.49 | 0.45 |
| 7:DC:417:ASN:HB3 | 7:DC:421:GLY:HA2 | 1.99 | 0.45 |
| 7:DB:418:ASP:OD2 | 7:DC:505:PRO:HD3 | 2.15 | 0.45 |
| 7:DD:101:SER:OG | 7:DD:105:GLU:HB2 | 2.17 | 0.45 |
| 7:DD:157:THR:OG1 | 7:DD:158:THR:N | 2.49 | 0.45 |
| 7:DD:36:ILE:O | 7:DD:39:ILE:HG13 | 2.17 | 0.45 |
| 8:DF:32:PHE:O | 8:DF:35:GLN:N | 2.50 | 0.45 |
| 3:E:76:MET:O | 3:E:299:PRO:HD3 | 2.16 | 0.45 |
| 1:EA:227:ARG:HB2 | 1:EA:237:TYR:HE2 | 1.81 | 0.45 |
| 1:EA:554:ILE:HG22 | 1:EA:555:ILE:O | 2.16 | 0.45 |
| 1:EB:104:SER:OG | 1:EB:316:GLY:O | 2.18 | 0.45 |
| 2:EC:191:TYR:HE2 | 2:EC:204:ARG:HB3 | 1.82 | 0.45 |
| 2:EC:347:GLU:CG | 2:EC:349:LEU:HD21 | 2.46 | 0.45 |
| 2:EC:483:LYS:HZ3 | 3:GH:228:ASN:HB2 | 1.82 | 0.45 |
| 2:EC:580:LYS:HG2 | 2:EC:581:TYR:N | 2.22 | 0.45 |
| 1:EA:79:PHE:CE1 | 2:EC:702:GLU:HG2 | 2.52 | 0.45 |
| 2:EC:878:ASP:O | 2:EC:881:ARG:N | 2.49 | 0.45 |
| 4:EF:67:TYR:CD1 | 4:EF:84:ARG:HB3 | 2.50 | 0.45 |
| 4:EH:8:LYS:HD2 | 4:EH:30:LYS:HA | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:214:SER:HB2 | 5:EI:225:LEU:HA | 1.99 | 0.45 |
| 5:EJ:3:GLN:HG3 | 5:EJ:25:LYS:HG3 | 1.97 | 0.45 |
| 4:F:145:LYS:N | 4:F:165:GLU:O | 2.49 | 0.45 |
| 5:FA:132:ASP:OD2 | 5:FA:151:ILE:HA | 2.16 | 0.45 |
| 5:EI:522:SER:C | 5:FA:591:PRO:HD3 | 2.37 | 0.45 |
| 7:FF:302:ILE:HD12 | 7:FG:306:PHE:CZ | 2.52 | 0.45 |
| 7:FF:417:ASN:HB3 | 7:FF:421:GLY:HA2 | 1.99 | 0.45 |
| 7:FF:418:ASP:HA | 7:FF:424:ARG:NH2 | 2.32 | 0.45 |
| 7:FG:36:ILE:O | 7:FG:39:ILE:HG13 | 2.17 | 0.45 |
| 4:G:68:GLN:HB3 | 4:G:70:HIS:NE2 | 2.32 | 0.45 |
| 1:GD:167:LEU:HA | 1:GD:167:LEU:HD23 | 1.76 | 0.45 |
| 1:GD:339:CYS:SG | 1:GD:400:ASN:HA | 2.57 | 0.45 |
| 1:GD:448:TYR:C | 1:GD:453:GLU:HG2 | 2.37 | 0.45 |
| 1:GD:81:ARG:HA | 1:GD:326:ARG:HG3 | 1.99 | 0.45 |
| 1:GE:182:LEU:HD12 | 1:GE:182:LEU:O | 2.16 | 0.45 |
| 1:GE:346:ASP:O | 1:GE:350:SER:N | 2.50 | 0.45 |
| 1:GE:472:ASP:OD2 | 1:GE:474:SER:HB2 | 2.17 | 0.45 |
| 2:GF:191:TYR:HE2 | 2:GF:204:ARG:HB3 | 1.82 | 0.45 |
| 2:GF:369:ASP:HB2 | 2:GF:434:MET:HG2 | 1.99 | 0.45 |
| 2:GF:527:ASN:OD1 | 2:GF:528:ASN:N | 2.50 | 0.45 |
| 2:GF:558:HIS:HB2 | 2:GF:569:VAL:HG12 | 1.99 | 0.45 |
| 2:GF:748:PHE:CD2 | 2:GF:756:VAL:HG11 | 2.52 | 0.45 |
| 3:GG:147:LEU:HD23 | 3:GG:149:ASP:N | 2.30 | 0.45 |
| 3:GG:46:PRO:HA | 3:GG:270:ARG:CZ | 2.47 | 0.45 |
| 2:EC:473:TYR:HB2 | 3:GG:59:PRO:HB2 | 1.99 | 0.45 |
| 5:HB:522:SER:C | 5:HD:591:PRO:HD3 | 2.37 | 0.45 |
| 5:HD:115:ASP:OD2 | 5:HD:137:TYR:HE1 | 2.00 | 0.45 |
| 5:HD:199:GLU:HG3 | 5:HD:200:LEU:N | 2.32 | 0.45 |
| 5:HD:192:ARG:HB2 | 5:HD:245:GLU:HB2 | 1.99 | 0.45 |
| 6:HG:203:LEU:HD12 | 6:HG:206:GLN:NE2 | 2.31 | 0.45 |
| 7:HI:117:THR:HG22 | 7:HI:120:LYS:NZ | 2.32 | 0.45 |
| 7:HI:170:ILE:HG23 | 7:HJ:173:ILE:HD13 | 1.98 | 0.45 |
| 7:HJ:36:ILE:O | 7:HJ:39:ILE:HG13 | 2.17 | 0.45 |
| 5:I:135:LEU:HA | 5:I:144:GLU:O | 2.17 | 0.45 |
| 5:I:554:GLY:O | 5:I:555:CYS:SG | 2.75 | 0.45 |
| 8:R:151:GLN:N | 8:IA:18:PRO:HD3 | 2.31 | 0.45 |
| 11:IE:186:ARG:HG2 | 11:IE:187:ILE:H | 1.82 | 0.45 |
| 5:J:288:MET:HE2 | 5:J:292:PRO:HD3 | 1.98 | 0.45 |
| 5:K:104:VAL:HG13 | 5:K:105:ASN:H | 1.80 | 0.45 |
| 5:J:249:ASP:CA | 5:K:158:ASP:HB3 | 2.47 | 0.45 |
| 7:O:12:GLU:HG3 | 7:O:14:ARG:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:513:ARG:N | 7:P:441:GLN:O | 2.34 | 0.45 |
| 7:P:478:ASP:CG | 7:Q:454:HIS:HE2 | 2.19 | 0.45 |
| 7:Q:123:VAL:O | 7:Q:127:ASN:N | 2.26 | 0.45 |
| 7:P:57:ILE:HG23 | 7:Q:56:GLY:CA | 2.47 | 0.45 |
| 7:Q:77:THR:HG23 | 7:Q:79:ALA:H | 1.79 | 0.45 |
| 12:W:184:PRO:HA | 12:IF:153:ARG:HH22 | 1.80 | 0.45 |
| 1:X:174:ARG:HH21 | 1:X:269:VAL:HG21 | 1.80 | 0.45 |
| 1:X:440:ILE:HG13 | 1:X:441:ILE:N | 2.31 | 0.45 |
| 1:X:448:TYR:C | 1:X:453:GLU:HG2 | 2.37 | 0.45 |
| 1:X:565:GLU:HB3 | 1:X:570:GLN:OE1 | 2.16 | 0.45 |
| 1:Y:197:VAL:HG11 | 1:Y:236:PHE:CZ | 2.52 | 0.45 |
| 13:YA:266[E]:TRP:CD1 | 13:YA:274[E]:GLN:HG2 | 2.51 | 0.45 |
| 13:YA:296[D]:LEU:HA | 13:YA:296[D]:LEU:HD12 | 1.85 | 0.45 |
| 13:YA:315[D]:LEU:O | 13:YA:319[D]:GLN:HG2 | 2.16 | 0.45 |
| 13:YA:407[E]:PRO:HB3 | 13:YC:232[E]:ASN:CB | 2.46 | 0.45 |
| 13:YA:490[B]:VAL:HG12 | 13:YA:492[B]:GLY:H | 1.81 | 0.45 |
| 13:YA:18[D]:ARG:CZ | 13:YA:77[D]:VAL:HG23 | 2.46 | 0.45 |
| 13:YB:110[D]:ARG:HD2 | 13:YB:118[D]:THR:O | 2.17 | 0.45 |
| 13:YB:110[A]:ARG:HD2 | 13:YB:118[A]:THR:O | 2.17 | 0.45 |
| 13:YA:66[E]:MET:HE2 | 13:YB:122[E]:PRO:HB3 | 1.98 | 0.45 |
| 13:YA:66[F]:MET:HE2 | 13:YB:122[F]:PRO:HB3 | 1.97 | 0.45 |
| 13:YB:236[B]:ILE:HG23 | 13:YB:240[B]:GLU:HB2 | 1.99 | 0.45 |
| 13:YB:261[A]:LYS:HE2 | 13:YB:293[A]:ASN:HB3 | 1.99 | 0.45 |
| 13:YA:70[B]:GLY:O | 13:YB:394[B]:GLU:N | 2.49 | 0.45 |
| 13:YB:67[D]:SER:HB3 | 13:YC:123[D]:ARG:HB2 | 1.98 | 0.45 |
| 13:YB:7[D]:ASN:HD22 | 13:YB:8[D]:LEU:HG | 1.82 | 0.45 |
| 13:YB:7[B]:ASN:HD22 | 13:YB:8[B]:LEU:HG | 1.81 | 0.45 |
| 13:YC:121[D]:TYR:OH | 13:YC:123[D]:ARG:NH2 | 2.50 | 0.45 |
| 13:YC:148[F]:GLN:NE2 | 13:YC:421[F]:TYR:OH | 2.49 | 0.45 |
| 13:YC:261[D]:LYS:HE2 | 13:YC:293[D]:ASN:HB3 | 1.99 | 0.45 |
| 13:YB:574[D]:ILE:HG22 | 13:YC:572[D]:ILE:HD13 | 1.97 | 0.45 |
| 13:YC:18[D]:ARG:CZ | 13:YC:77[D]:VAL:HG23 | 2.46 | 0.45 |
| 14:YD:15[C]:LYS:HE2 | 14:YD:15[C]:LYS:HB3 | 1.53 | 0.45 |
| 14:YD:73[D]:SER:HB2 | 14:YD:85[D]:THR:HG23 | 1.99 | 0.45 |
| 14:YE:117[A]:ASN:O | 14:YE:119[A]:LYS:HG3 | 2.16 | 0.45 |
| 14:YE:127[A]:ASP:CG | 14:YE:130[A]:GLU:H | 2.20 | 0.45 |
| 14:YE:160[A]:ILE:HG21 | 14:YE:282[A]:ALA:HB1 | 1.98 | 0.45 |
| 14:YE:135[A]:MET:SD | 14:YE:166[A]:PHE:HD1 | 2.40 | 0.45 |
| 14:YE:242[D]:PRO:HD2 | 14:YF:91[D]:LYS:O | 2.17 | 0.45 |
| 14:YE:266[D]:ILE:HD11 | 14:YE:290[D]:ASN:CG | 2.37 | 0.45 |
| 14:YE:266[F]:ILE:HD11 | 14:YE:290[F]:ASN:CG | 2.36 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:279[C]:ARG:HD3 | 14:YE:279[C]:ARG:HA | 1.43 | 0.45 |
| 14:YE:277[E]:VAL:HG11 | 14:YE:294[E]:GLU:HG2 | 1.98 | 0.45 |
| 14:YE:307[C]:TYR:HA | 14:YE:307[C]:TYR:HD1 | 1.66 | 0.45 |
| 14:YE:73[A]:SER:HB2 | 14:YE:85[A]:THR:HG23 | 1.99 | 0.45 |
| 14:YF:117[D]:ASN:O | 14:YF:119[D]:LYS:HG3 | 2.16 | 0.45 |
| 14:YF:170[B]:LEU:HA | 14:YF:170[B]:LEU:HD23 | 1.69 | 0.45 |
| 14:YF:178[B]:LEU:CD1 | 14:YF:183[B]:ASP:HA | 2.45 | 0.45 |
| 14:YF:336[D]:GLU:O | 14:YF:359[D]:THR:OG1 | 2.33 | 0.45 |
| 14:YF:73[F]:SER:HB2 | 14:YF:85[F]:THR:HG23 | 1.99 | 0.45 |
| 15:ZA:66[B]:LYS:O | 15:ZA:68[B]:TYR:HD1 | 1.99 | 0.45 |
| 1:A:106:ALA:HB3 | 1:A:169:GLN:HB2 | 1.98 | 0.45 |
| 1:A:277:GLY:O | 1:A:279:ASP:N | 2.50 | 0.45 |
| 4:AA:68:GLN:HB3 | 4:AA:70:HIS:NE2 | 2.32 | 0.45 |
| 4:AB:68:GLN:HB3 | 4:AB:70:HIS:NE2 | 2.32 | 0.45 |
| 5:AC:118:LYS:HZ3 | 5:AC:147:LYS:HD3 | 1.82 | 0.45 |
| 5:AC:133:LEU:HA | 5:AC:133:LEU:HD23 | 1.80 | 0.45 |
| 5:AC:20:ARG:NH1 | 5:AC:24:ILE:HD12 | 2.32 | 0.45 |
| 5:AC:290:SER:HA | 5:AC:371:PHE:H | 1.82 | 0.45 |
| 5:AC:293:PHE:HA | 5:AC:295:ALA:H | 1.82 | 0.45 |
| 5:AC:318:GLN:HB3 | 6:AH:4:LEU:HD12 | 1.99 | 0.45 |
| 5:AC:45:SER:OG | 5:AE:66:LYS:HA | 2.17 | 0.45 |
| 5:AC:98:VAL:HG11 | 5:AE:89:TYR:HB3 | 1.98 | 0.45 |
| 5:AD:120:SER:OG | 5:AD:122:VAL:HG22 | 2.16 | 0.45 |
| 5:AD:260:ARG:HA | 5:AD:384:THR:HA | 1.98 | 0.45 |
| 5:AE:393:LEU:O | 5:AE:394:LEU:HB2 | 2.16 | 0.45 |
| 6:AF:203:LEU:HD12 | 6:AF:206:GLN:NE2 | 2.31 | 0.45 |
| 6:AG:107:VAL:HG22 | 6:AG:174:TYR:HD2 | 1.82 | 0.45 |
| 6:AH:107:VAL:HG22 | 6:AH:174:TYR:HD2 | 1.82 | 0.45 |
| 7:AI:132:ARG:O | 7:AI:141:VAL:HG12 | 2.17 | 0.45 |
| 7:AI:447:HIS:CD2 | 7:BA:447:HIS:CD2 | 3.05 | 0.45 |
| 5:AC:196:ARG:HH11 | 7:AI:5:THR:CG2 | 2.29 | 0.45 |
| 7:AI:77:THR:OG1 | 7:AI:78:PRO:HD2 | 2.16 | 0.45 |
| 1:B:188:TYR:HD1 | 1:B:233:ASN:ND2 | 2.15 | 0.45 |
| 1:B:349:VAL:HG13 | 1:B:392:ILE:HD11 | 1.98 | 0.45 |
| 1:B:374:ILE:HB | 1:B:408:ILE:HG12 | 1.98 | 0.45 |
| 1:B:538:VAL:HG11 | 1:B:558:PHE:HE1 | 1.80 | 0.45 |
| 7:AJ:170:ILE:HG23 | 7:BA:173:ILE:HD13 | 1.97 | 0.45 |
| 7:AI:401:ARG:NH2 | 7:BA:397:GLY:O | 2.49 | 0.45 |
| 7:AI:485:ASN:OD1 | 7:BA:448:ALA:N | 2.49 | 0.45 |
| 8:BB:70:THR:HG22 | 8:BB:156:THR:HG22 | 1.98 | 0.45 |
| 11:BF:14:LYS:O | 11:BF:15:THR:HG22 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:BF:73:LEU:HD22 | 11:BF:86:TRP:CH2 | 2.52 | 0.45 |
| 1:BH:642:PHE:HE1 | 1:BH:651:LEU:HD13 | 1.82 | 0.45 |
| 1:BH:440:ILE:HD11 | 1:BH:653:ILE:HG21 | 1.98 | 0.45 |
| 1:BH:654:ASP:OD1 | 1:BH:655:LEU:N | 2.49 | 0.45 |
| 1:BI:90:VAL:O | 1:BI:94:GLN:HG2 | 2.17 | 0.45 |
| 2:BJ:191:TYR:HE2 | 2:BJ:204:ARG:HB3 | 1.82 | 0.45 |
| 2:BJ:244:THR:HB | 2:BJ:246:TYR:CZ | 2.51 | 0.45 |
| 2:C:546:GLU:N | 2:C:546:GLU:OE1 | 2.49 | 0.45 |
| 4:CC:168:PHE:CE1 | 4:CD:149:ARG:HB3 | 2.52 | 0.45 |
| 4:CE:8:LYS:HD2 | 4:CE:30:LYS:HA | 1.98 | 0.45 |
| 5:CF:214:SER:HB2 | 5:CF:225:LEU:HA | 1.99 | 0.45 |
| 5:CF:54:ALA:HB2 | 5:CF:71:ASN:O | 2.16 | 0.45 |
| 5:CF:60:LEU:CG | 5:CF:79:ILE:HG22 | 2.46 | 0.45 |
| 5:CH:158:ASP:OD1 | 5:CH:159:ILE:N | 2.47 | 0.45 |
| 5:CH:192:ARG:HB2 | 5:CH:245:GLU:HB2 | 1.99 | 0.45 |
| 6:CI:107:VAL:HG22 | 6:CI:174:TYR:HD2 | 1.82 | 0.45 |
| 3:D:147:LEU:HD11 | 3:D:152:GLU:CD | 2.37 | 0.45 |
| 6:CJ:69:THR:HA | 6:DA:73:ASN:CB | 2.46 | 0.45 |
| 7:DB:185:GLU:HA | 7:DD:193:LEU:HB2 | 1.98 | 0.45 |
| 7:DB:453:GLU:CD | 7:DB:471:THR:H | 2.18 | 0.45 |
| 7:DD:100:TYR:CE1 | 7:DD:115:SER:HB2 | 2.52 | 0.45 |
| 7:DD:359:TRP:CZ2 | 7:DD:524:LYS:HD3 | 2.52 | 0.45 |
| 7:DD:493:GLU:HA | 7:DD:496:ARG:NH2 | 2.32 | 0.45 |
| 11:DI:5:PHE:CE2 | 11:DI:188:MET:HG2 | 2.52 | 0.45 |
| 1:EA:440:ILE:HG13 | 1:EA:441:ILE:N | 2.31 | 0.45 |
| 1:EB:50:GLY:HA2 | 2:EC:657:TYR:OH | 2.16 | 0.45 |
| 1:EB:424:TYR:HE2 | 1:EB:655:LEU:HD13 | 1.81 | 0.45 |
| 1:EA:67:ILE:CD1 | 1:EB:67:ILE:HG21 | 2.47 | 0.45 |
| 1:EB:90:VAL:O | 1:EB:94:GLN:HG2 | 2.17 | 0.45 |
| 2:EC:110:PHE:HB3 | 2:EC:621:ALA:HA | 1.99 | 0.45 |
| 2:EC:479:TRP:CD1 | 2:EC:505:PRO:O | 2.70 | 0.45 |
| 2:EC:541:TYR:CG | 2:EC:542:THR:N | 2.85 | 0.45 |
| 2:EC:546:GLU:OE1 | 2:EC:546:GLU:N | 2.49 | 0.45 |
| 2:EC:558:HIS:HB2 | 2:EC:569:VAL:HG12 | 1.99 | 0.45 |
| 1:EA:341:THR:HG23 | 2:EC:880:ILE:O | 2.17 | 0.45 |
| 3:ED:93:ARG:HH21 | 3:ED:106:PHE:HD1 | 1.64 | 0.45 |
| 4:EF:68:GLN:HB3 | 4:EF:70:HIS:NE2 | 2.32 | 0.45 |
| 5:EJ:120:SER:OG | 5:EJ:122:VAL:HG22 | 2.16 | 0.45 |
| 5:FA:192:ARG:HB2 | 5:FA:245:GLU:HB2 | 1.99 | 0.45 |
| 5:FA:310:GLU:HB2 | 5:FA:384:THR:CB | 2.47 | 0.45 |
| 5:FA:310:GLU:HB2 | 5:FA:384:THR:HB | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:377:HIS:CG | 5:FA:378:GLY:N | 2.85 | 0.45 |
| 5:FA:393:LEU:O | 5:FA:394:LEU:HB2 | 2.16 | 0.45 |
| 5:EI:49:TRP:HB2 | 5:FA:90:ASN:OD1 | 2.17 | 0.45 |
| 7:FE:101:SER:HA | 7:FE:105:GLU:OE1 | 2.16 | 0.45 |
| 7:FE:12:GLU:HG3 | 7:FE:14:ARG:N | 2.31 | 0.45 |
| 7:FF:228:ILE:HG21 | 7:FF:244:ALA:HB2 | 1.97 | 0.45 |
| 7:FF:99:ARG:HG2 | 7:FF:100:TYR:O | 2.17 | 0.45 |
| 7:FF:445:HIS:CE1 | 7:FG:447:HIS:CE1 | 3.05 | 0.45 |
| 8:FH:114:ARG:HD2 | 8:FH:123:VAL:HG11 | 1.97 | 0.45 |
| 8:R:99:ILE:HD11 | 8:FH:55:ASN:HB3 | 1.97 | 0.45 |
| 4:G:201:LYS:NZ | 4:G:220:ASN:OD1 | 2.37 | 0.45 |
| 12:GC:122:GLY:O | 12:GC:125:ILE:HG22 | 2.17 | 0.45 |
| 12:GC:24:CYS:CB | 12:GC:125:ILE:HD13 | 2.47 | 0.45 |
| 1:GE:219:SER:O | 1:GE:220:THR:OG1 | 2.29 | 0.45 |
| 1:GE:206:TRP:CE2 | 1:GE:222:THR:HB | 2.52 | 0.45 |
| 1:GE:470:ASP:O | 1:GE:472:ASP:N | 2.50 | 0.45 |
| 1:GD:67:ILE:CD1 | 1:GE:67:ILE:HG21 | 2.47 | 0.45 |
| 2:GF:347:GLU:CG | 2:GF:349:LEU:HD21 | 2.46 | 0.45 |
| 2:GF:437:ASP:OD1 | 2:GF:440:LEU:HB2 | 2.16 | 0.45 |
| 2:GF:724:ALA:O | 2:GF:725:ARG:HG2 | 2.17 | 0.45 |
| 4:GJ:113:ASN:ND2 | 4:HA:103:LEU:HD21 | 2.27 | 0.45 |
| 4:HA:68:GLN:HB3 | 4:HA:70:HIS:NE2 | 2.32 | 0.45 |
| 5:HB:135:LEU:HA | 5:HB:144:GLU:O | 2.17 | 0.45 |
| 5:HB:153:LYS:HE3 | 5:HB:155:THR:OG1 | 2.17 | 0.45 |
| 5:HC:221:GLU:N | 5:HC:221:GLU:OE1 | 2.49 | 0.45 |
| 5:HC:3:GLN:HG3 | 5:HC:25:LYS:HG3 | 1.98 | 0.45 |
| 5:HD:469:PRO:HA | 5:HD:472:TYR:CZ | 2.52 | 0.45 |
| 5:HD:563:GLY:N | 5:HD:564:PRO:HD3 | 2.31 | 0.45 |
| 6:HE:57:ASN:HB2 | 6:HF:164:GLN:NE2 | 2.31 | 0.45 |
| 7:HH:147:LEU:HB2 | 7:HH:148:PRO:HD3 | 1.97 | 0.45 |
| 7:HH:405:ARG:NH2 | 7:HH:409:LEU:O | 2.49 | 0.45 |
| 7:HH:509:GLY:HA3 | 7:HI:441:GLN:HE21 | 1.82 | 0.45 |
| 7:HI:66:VAL:HG11 | 7:HI:80:THR:HB | 1.98 | 0.45 |
| 7:HJ:101:SER:OG | 7:HJ:105:GLU:HB2 | 2.17 | 0.45 |
| 8:IA:122:THR:HG22 | 8:IA:123:VAL:H | 1.81 | 0.45 |
| 8:IA:79:HIS:HE1 | 8:IA:151:GLN:HE22 | 1.63 | 0.45 |
| 10:ID:203:ARG:NH2 | 10:ID:356:ARG:HH12 | 2.13 | 0.45 |
| 11:IE:88:THR:HG22 | 11:IE:92:ALA:HB3 | 1.99 | 0.45 |
| 12:IF:195:VAL:O | 12:IF:195:VAL:HG12 | 2.16 | 0.45 |
| 12:IF:220:SER:HA | 12:IF:243:PHE:HD1 | 1.82 | 0.45 |
| 5:J:395:THR:HG22 | 5:K:307:ASN:HD21 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:K:115:ASP:OD2 | 5:K:137:TYR:HE1 | 2.00 | 0.45 |
| 5:K:304:ILE:HD11 | 5:K:366:PRO:HG3 | 1.99 | 0.45 |
| 5:K:71:ASN:OD1 | 5:K:73:SER:N | 2.32 | 0.45 |
| 7:O:405:ARG:NH2 | 7:O:409:LEU:O | 2.49 | 0.45 |
| 7:Q:63:GLU:O | 7:Q:67:ILE:HG12 | 2.16 | 0.45 |
| 8:R:3:VAL:HG12 | 8:S:58:ILE:HG23 | 1.98 | 0.45 |
| 8:S:70:THR:HG22 | 8:S:156:THR:HG22 | 1.98 | 0.45 |
| 9:T:10:ASP:O | 9:T:26:SER:N | 2.48 | 0.45 |
| 1:X:339:CYS:SG | 1:X:400:ASN:HA | 2.57 | 0.45 |
| 1:Y:200:TYR:HB2 | 1:Y:269:VAL:HG13 | 1.97 | 0.45 |
| 1:Y:386:THR:HG23 | 1:Y:387:VAL:N | 2.31 | 0.45 |
| 1:Y:563:VAL:HG12 | 1:Y:564:THR:O | 2.15 | 0.45 |
| 13:YA:110[F]:ARG:HD2 | 13:YA:118[F]:THR:O | 2.17 | 0.45 |
| 13:YA:236[B]:ILE:HG23 | 13:YA:240[B]:GLU:HB2 | 1.99 | 0.45 |
| 13:YA:315[A]:LEU:O | 13:YA:319[A]:GLN:HG2 | 2.16 | 0.45 |
| 13:YA:416[C]:HIS:CG | 13:YA:417[C]:PRO:HD2 | 2.51 | 0.45 |
| 13:YA:498[F]:VAL:HA | 13:YB:490[F]:VAL:O | 2.17 | 0.45 |
| 13:YA:521[E]:LEU:HD12 | 13:YA:522[E]:VAL:N | 2.32 | 0.45 |
| 13:YA:534[B]:LEU:CB | 13:YC:538[B]:VAL:HG11 | 2.46 | 0.45 |
| 13:YA:558[C]:SER:O | 13:YB:551[C]:THR:HA | 2.16 | 0.45 |
| 13:YB:180[E]:LEU:HA | 13:YB:180[E]:LEU:HD13 | 1.76 | 0.45 |
| 13:YB:315[E]:LEU:O | 13:YB:319[E]:GLN:HG2 | 2.16 | 0.45 |
| 13:YA:315[D]:LEU:HD23 | 13:YB:367[D]:PRO:HA | 1.97 | 0.45 |
| 13:YA:498[D]:VAL:HA | 13:YB:490[D]:VAL:O | 2.16 | 0.45 |
| 13:YA:498[E]:VAL:HA | 13:YB:490[E]:VAL:O | 2.17 | 0.45 |
| 13:YB:521[C]:LEU:HD12 | 13:YB:522[C]:VAL:N | 2.32 | 0.45 |
| 13:YB:534[E]:LEU:HD11 | 13:YB:536[E]:TRP:NE1 | 2.32 | 0.45 |
| 13:YB:553[C]:LYS:HB2 | 13:YB:553[C]:LYS:HZ2 | 1.82 | 0.45 |
| 13:YB:561[D]:SER:HA | 13:YC:554[D]:MET:O | 2.16 | 0.45 |
| 13:YB:7[F]:ASN:HD22 | 13:YB:8[F]:LEU:HG | 1.82 | 0.45 |
| 13:YB:24[F]:LEU:HD21 | 13:YC:102[F]:GLY:HA2 | 1.98 | 0.45 |
| 13:YC:110[D]:ARG:HD2 | 13:YC:118[D]:THR:O | 2.17 | 0.45 |
| 13:YB:73[D]:VAL:HG21 | 13:YC:129[D]:THR:HG22 | 1.99 | 0.45 |
| 13:YC:252[C]:MET:HE3 | 13:YC:252[C]:MET:HB3 | 1.83 | 0.45 |
| 13:YC:261[F]:LYS:HE2 | 13:YC:293[F]:ASN:HB3 | 1.99 | 0.45 |
| 13:YC:296[D]:LEU:HD12 | 13:YC:296[D]:LEU:HA | 1.85 | 0.45 |
| 13:YC:315[C]:LEU:O | 13:YC:319[C]:GLN:HG2 | 2.16 | 0.45 |
| 13:YC:416[E]:HIS:CG | 13:YC:417[E]:PRO:HD2 | 2.51 | 0.45 |
| 13:YC:490[D]:VAL:HG12 | 13:YC:492[D]:GLY:H | 1.82 | 0.45 |
| 13:YC:521[A]:LEU:HD12 | 13:YC:522[A]:VAL:N | 2.32 | 0.45 |
| 14:YD:117[D]:ASN:O | 14:YD:119[D]:LYS:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:266[A]:ILE:HD11 | 14:YD:290[A]:ASN:CG | 2.36 | 0.45 |
| 14:YD:97[D]:VAL:HG12 | 14:YF:234[D]:PHE:HD1 | 1.82 | 0.45 |
| 14:YE:117[F]:ASN:O | 14:YE:119[F]:LYS:HG3 | 2.17 | 0.45 |
| 14:YE:20[D]:TYR:HA | 14:YE:69[D]:ILE:HD12 | 1.99 | 0.45 |
| 14:YF:117[F]:ASN:O | 14:YF:119[F]:LYS:HG3 | 2.17 | 0.45 |
| 14:YF:160[C]:ILE:HG21 | 14:YF:282[C]:ALA:HB1 | 1.98 | 0.45 |
| 14:YF:212[A]:ILE:HG22 | 14:YF:327[A]:ASN:HB2 | 1.98 | 0.45 |
| 14:YF:266[E]:ILE:HD11 | 14:YF:290[E]:ASN:CG | 2.37 | 0.45 |
| 14:YF:288[F]:TYR:CE1 | 14:YF:371[F]:LYS:HD3 | 2.52 | 0.45 |
| 14:YE:236[B]:TRP:N | 14:YF:95[B]:VAL:O | 2.50 | 0.45 |
| 2:Z:110:PHE:HB3 | 2:Z:621:ALA:HA | 1.99 | 0.45 |
| 2:Z:244:THR:HB | 2:Z:246:TYR:CZ | 2.51 | 0.45 |
| 2:Z:437:ASP:OD1 | 2:Z:440:LEU:HB2 | 2.16 | 0.45 |
| 2:Z:146:LEU:HD11 | 2:Z:578:PHE:CE1 | 2.51 | 0.45 |
| 2:Z:796:THR:HG23 | 2:Z:797:TYR:CD2 | 2.52 | 0.45 |
| 1:A:544:ASP:HB2 | 1:A:576:ASP:OD2 | 2.16 | 0.45 |
| 1:A:60:LEU:HD13 | 2:C:671:TYR:CD1 | 2.52 | 0.45 |
| 4:AB:111:ASN:HB2 | 4:AB:116:ILE:HD12 | 1.98 | 0.45 |
| 5:AC:10:VAL:HG23 | 5:AC:11:VAL:HG23 | 1.97 | 0.45 |
| 5:AC:402:GLU:HG3 | 5:AC:406:LEU:CD1 | 2.47 | 0.45 |
| 5:AD:206:PHE:HB3 | 5:AD:223:VAL:HG13 | 1.99 | 0.45 |
| 5:AC:386:PHE:CZ | 5:AD:390:LEU:HD13 | 2.52 | 0.45 |
| 5:AD:466:PRO:HA | 5:AD:596:TYR:CZ | 2.52 | 0.45 |
| 5:AC:591:PRO:HD3 | 5:AD:522:SER:C | 2.37 | 0.45 |
| 5:AE:199:GLU:HG3 | 5:AE:200:LEU:N | 2.32 | 0.45 |
| 5:AE:202:TYR:CE1 | 5:AE:206:PHE:HD1 | 2.35 | 0.45 |
| 6:AH:87:TYR:N | 6:AH:181:GLU:O | 2.32 | 0.45 |
| 7:AJ:32:VAL:HG22 | 7:AJ:36:ILE:HG12 | 1.99 | 0.45 |
| 7:AI:509:GLY:HA3 | 7:AJ:441:GLN:HE21 | 1.82 | 0.45 |
| 7:AJ:59:PHE:CZ | 7:BA:55:LYS:HG3 | 2.52 | 0.45 |
| 1:B:472:ASP:OD2 | 1:B:474:SER:HB2 | 2.17 | 0.45 |
| 8:BB:32:PHE:O | 8:BB:35:GLN:N | 2.50 | 0.45 |
| 9:BD:96:ILE:O | 9:BD:105:ILE:HG22 | 2.17 | 0.45 |
| 11:BF:186:ARG:HG2 | 11:BF:187:ILE:H | 1.82 | 0.45 |
| 1:BH:172:ILE:HD13 | 1:BH:273:ILE:HG12 | 1.99 | 0.45 |
| 1:BH:444:ILE:O | 1:BH:447:TYR:HB3 | 2.16 | 0.45 |
| 1:BI:106:ALA:HB2 | 1:BI:280:ALA:CB | 2.45 | 0.45 |
| 1:BI:538:VAL:HG11 | 1:BI:558:PHE:HE1 | 1.80 | 0.45 |
| 2:BJ:37:GLU:O | 2:BJ:80:ILE:HA | 2.17 | 0.45 |
| 2:BJ:527:ASN:OD1 | 2:BJ:528:ASN:N | 2.50 | 0.45 |
| 2:BJ:761:GLU:HB2 | 2:BJ:862:TYR:CZ | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:549:PRO:HB2 | 2:C:550:GLU:OE1 | 2.17 | 0.45 |
| 3:CB:199:SER:OG | 3:CB:200:ILE:N | 2.50 | 0.45 |
| 5:CF:323:THR:HG21 | 5:CF:354:THR:HG23 | 1.98 | 0.45 |
| 5:CG:395:THR:HG22 | 5:CH:307:ASN:HD21 | 1.82 | 0.45 |
| 5:CH:470:VAL:O | 5:CH:474:GLY:N | 2.50 | 0.45 |
| 5:CF:518:GLY:N | 5:CH:594:THR:OG1 | 2.49 | 0.45 |
| 3:D:64:SER:HG | 3:D:67:GLY:H | 1.58 | 0.45 |
| 7:DB:283:TRP:CZ3 | 7:DB:284:ASN:HB3 | 2.52 | 0.45 |
| 7:DB:468:PHE:HB2 | 7:DD:479:ASN:O | 2.16 | 0.45 |
| 7:DB:87:TYR:HB3 | 7:DB:88:PRO:HD3 | 1.99 | 0.45 |
| 7:DC:45:ASN:CG | 7:DD:24:ASN:HD21 | 2.19 | 0.45 |
| 7:DB:472:ARG:NH1 | 7:DD:474:GLY:HA2 | 2.31 | 0.45 |
| 12:DJ:144:ASN:ND2 | 10:GA:57:LEU:HG | 2.32 | 0.45 |
| 3:E:204:THR:O | 3:E:207:TYR:N | 2.49 | 0.45 |
| 3:E:72:TRP:HZ3 | 3:E:275:ILE:CD1 | 2.29 | 0.45 |
| 1:EA:339:CYS:SG | 1:EA:400:ASN:HA | 2.57 | 0.45 |
| 1:EA:596:ASN:N | 1:EA:596:ASN:OD1 | 2.47 | 0.45 |
| 2:EC:138:ASN:O | 2:EC:555:ARG:CZ | 2.64 | 0.45 |
| 2:EC:168:ILE:HA | 2:EC:168:ILE:HD12 | 1.88 | 0.45 |
| 2:EC:209:VAL:O | 2:EC:221:ALA:HA | 2.16 | 0.45 |
| 2:EC:479:TRP:CG | 2:EC:505:PRO:O | 2.69 | 0.45 |
| 2:EC:527:ASN:OD1 | 2:EC:528:ASN:N | 2.50 | 0.45 |
| 2:EC:982:LEU:HD12 | 2:EC:982:LEU:O | 2.17 | 0.45 |
| 3:EE:106:PHE:CD2 | 3:EE:188:TRP:HH2 | 2.35 | 0.45 |
| 3:EE:40:THR:OG1 | 3:EE:273:SER:HB3 | 2.17 | 0.45 |
| 4:EG:111:ASN:HB2 | 4:EG:116:ILE:HD12 | 1.98 | 0.45 |
| 4:EG:1:MET:HG2 | 4:EG:70:HIS:ND1 | 2.32 | 0.45 |
| 4:EH:68:GLN:HB3 | 4:EH:70:HIS:NE2 | 2.32 | 0.45 |
| 5:EI:135:LEU:HA | 5:EI:144:GLU:O | 2.17 | 0.45 |
| 5:EI:118:LYS:HZ3 | 5:EI:147:LYS:HD3 | 1.82 | 0.45 |
| 5:EI:153:LYS:HE3 | 5:EI:155:THR:OG1 | 2.17 | 0.45 |
| 5:EI:402:GLU:HG3 | 5:EI:406:LEU:CD1 | 2.47 | 0.45 |
| 5:FA:469:PRO:HA | 5:FA:472:TYR:CZ | 2.52 | 0.45 |
| 6:FC:86:ASP:CG | 6:FC:180:GLN:HE21 | 2.19 | 0.45 |
| 7:FE:147:LEU:HB2 | 7:FE:148:PRO:HD3 | 1.98 | 0.45 |
| 7:FE:382:ARG:HG3 | 7:FE:383:TYR:CD2 | 2.52 | 0.45 |
| 7:FE:87:TYR:HB3 | 7:FE:88:PRO:HD3 | 1.99 | 0.45 |
| 7:FF:216:MET:SD | 7:FG:202:GLY:HA3 | 2.56 | 0.45 |
| 7:FG:493:GLU:HA | 7:FG:496:ARG:NH2 | 2.32 | 0.45 |
| 1:GE:23:GLY:O | 1:GE:29:ILE:HD11 | 2.15 | 0.45 |
| 1:GE:502:ASN:OD1 | 1:GE:635:ARG:NH2 | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:1020:ARG:NH2 | 3:GG:94:ASP:OD2 | 2.50 | 0.45 |
| 3:GG:93:ARG:HH21 | 3:GG:106:PHE:HD1 | 1.64 | 0.45 |
| 3:GG:71:MET:HE1 | 3:GG:271:GLN:HG2 | 1.98 | 0.45 |
| 2:GF:911:THR:HG23 | 3:GG:330:ILE:HG12 | 1.98 | 0.45 |
| 3:GH:40:THR:OG1 | 3:GH:273:SER:HB3 | 2.17 | 0.45 |
| 4:GI:68:GLN:HB3 | 4:GI:70:HIS:NE2 | 2.32 | 0.45 |
| 4:GJ:8:LYS:HD2 | 4:GJ:30:LYS:HA | 1.98 | 0.45 |
| 4:H:1:MET:HG2 | 4:H:70:HIS:ND1 | 2.32 | 0.45 |
| 4:GI:222:LEU:HD13 | 4:HA:216:THR:HG23 | 1.98 | 0.45 |
| 5:HB:20:ARG:NH1 | 5:HB:24:ILE:HD12 | 2.32 | 0.45 |
| 5:HC:503:ASN:OD1 | 5:HC:504:ASN:N | 2.49 | 0.45 |
| 5:HD:202:TYR:CE1 | 5:HD:206:PHE:HD1 | 2.35 | 0.45 |
| 5:HC:395:THR:HG22 | 5:HD:307:ASN:HD21 | 1.81 | 0.45 |
| 5:HD:310:GLU:HB2 | 5:HD:384:THR:CB | 2.47 | 0.45 |
| 6:HG:107:VAL:HG22 | 6:HG:174:TYR:HD2 | 1.82 | 0.45 |
| 7:HH:39:ILE:HA | 7:HJ:44:VAL:HG22 | 1.98 | 0.45 |
| 7:HI:111:ASN:ND2 | 7:HI:114:SER:HB3 | 2.32 | 0.45 |
| 7:HH:485:ASN:OD1 | 7:HJ:448:ALA:N | 2.50 | 0.45 |
| 5:I:85:THR:HB | 5:I:137:TYR:CE2 | 2.52 | 0.45 |
| 10:ID:37:GLN:HB3 | 10:ID:128:LEU:HB3 | 1.99 | 0.45 |
| 12:IF:127:SER:HB3 | 12:IF:161:SER:HG | 1.81 | 0.45 |
| 5:K:103:ASN:CG | 5:K:104:VAL:H | 2.20 | 0.45 |
| 5:K:131:SER:HA | 5:K:150:GLN:HA | 1.99 | 0.45 |
| 5:K:267:ASP:CG | 5:K:377:HIS:HA | 2.37 | 0.45 |
| 5:K:310:GLU:HB2 | 5:K:384:THR:CB | 2.47 | 0.45 |
| 5:K:470:VAL:O | 5:K:474:GLY:N | 2.49 | 0.45 |
| 6:L:86:ASP:CG | 6:L:180:GLN:HE21 | 2.19 | 0.45 |
| 6:M:144:ASN:HB3 | 6:M:159:THR:HG22 | 1.99 | 0.45 |
| 5:K:316:ILE:HD13 | 6:M:7:LYS:HG3 | 1.98 | 0.45 |
| 7:O:462:ASN:HB3 | 7:Q:482:TYR:HD1 | 1.82 | 0.45 |
| 7:P:117:THR:HG22 | 7:P:120:LYS:NZ | 2.32 | 0.45 |
| 7:P:66:VAL:HG11 | 7:P:80:THR:HB | 1.98 | 0.45 |
| 7:Q:36:ILE:O | 7:Q:39:ILE:HG13 | 2.17 | 0.45 |
| 8:R:122:THR:HG22 | 8:R:123:VAL:H | 1.81 | 0.45 |
| 11:V:186:ARG:HG2 | 11:V:187:ILE:H | 1.82 | 0.45 |
| 1:X:229:THR:OG1 | 1:X:233:ASN:O | 2.35 | 0.45 |
| 1:X:642:PHE:HE1 | 1:X:651:LEU:HD13 | 1.82 | 0.45 |
| 2:C:720:ARG:HD2 | 1:Y:430:GLN:NE2 | 2.31 | 0.45 |
| 13:YA:110[C]:ARG:HD2 | 13:YA:118[C]:THR:O | 2.17 | 0.45 |
| 13:YA:121[D]:TYR:OH | 13:YA:123[D]:ARG:NH2 | 2.50 | 0.45 |
| 13:YA:315[F]:LEU:O | 13:YA:319[F]:GLN:HG2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:543[D]:ASP:HA | 13:YC:551[D]:THR:O | 2.17 | 0.45 |
| 13:YB:110[F]:ARG:HD2 | 13:YB:118[F]:THR:O | 2.17 | 0.45 |
| 13:YB:180[D]:LEU:HD13 | 13:YB:180[D]:LEU:HA | 1.76 | 0.45 |
| 13:YB:416[A]:HIS:CG | 13:YB:417[A]:PRO:HD2 | 2.51 | 0.45 |
| 13:YB:521[A]:LEU:HD12 | 13:YB:522[A]:VAL:N | 2.32 | 0.45 |
| 13:YB:521[D]:LEU:HD12 | 13:YB:522[D]:VAL:N | 2.32 | 0.45 |
| 13:YB:7[A]:ASN:HD22 | 13:YB:8[A]:LEU:HG | 1.82 | 0.45 |
| 13:YC:236[F]:ILE:HG23 | 13:YC:240[F]:GLU:HB2 | 1.99 | 0.45 |
| 13:YC:257[F]:LYS:HE2 | 13:YC:266[F]:TRP:CH2 | 2.52 | 0.45 |
| 13:YC:296[C]:LEU:HA | 13:YC:296[C]:LEU:HD12 | 1.84 | 0.45 |
| 13:YC:521[E]:LEU:HD12 | 13:YC:522[E]:VAL:N | 2.32 | 0.45 |
| 13:YC:537[A]:LYS:HD3 | 13:YC:537[A]:LYS:C | 2.37 | 0.45 |
| 14:YD:117[C]:ASN:O | 14:YD:119[C]:LYS:HG3 | 2.16 | 0.45 |
| 14:YD:160[A]:ILE:HG21 | 14:YD:282[A]:ALA:HB1 | 1.98 | 0.45 |
| 14:YD:135[D]:MET:SD | 14:YD:166[D]:PHE:HD1 | 2.39 | 0.45 |
| 14:YD:178[A]:LEU:CD1 | 14:YD:183[A]:ASP:HA | 2.45 | 0.45 |
| 14:YD:266[B]:ILE:HD11 | 14:YD:290[B]:ASN:CG | 2.36 | 0.45 |
| 14:YD:266[D]:ILE:HD11 | 14:YD:290[D]:ASN:CG | 2.37 | 0.45 |
| 14:YD:236[A]:TRP:CD1 | 14:YD:308[A]:ALA:HB2 | 2.51 | 0.45 |
| 14:YD:20[E]:TYR:HA | 14:YD:69[E]:ILE:HD12 | 1.99 | 0.45 |
| 14:YD:97[F]:VAL:HG12 | 14:YF:234[F]:PHE:HD1 | 1.82 | 0.45 |
| 14:YE:140[F]:TYR:HE2 | 14:YE:148[F]:PRO:HD3 | 1.82 | 0.45 |
| 14:YE:15[A]:LYS:HE2 | 14:YE:15[A]:LYS:HB3 | 1.54 | 0.45 |
| 14:YE:178[E]:LEU:CD1 | 14:YE:183[E]:ASP:HA | 2.45 | 0.45 |
| 11:IE:175:SER:HA | 14:YE:217[D]:SER:HB2 | 1.97 | 0.45 |
| 14:YE:242[F]:PRO:HD2 | 14:YF:91[F]:LYS:O | 2.17 | 0.45 |
| 14:YE:277[F]:VAL:HG11 | 14:YE:294[F]:GLU:HG2 | 1.99 | 0.45 |
| 14:YE:279[B]:ARG:HD3 | 14:YE:279[B]:ARG:HA | 1.43 | 0.45 |
| 14:YE:307[A]:TYR:HD1 | 14:YE:307[A]:TYR:HA | 1.66 | 0.45 |
| 14:YE:236[B]:TRP:CD1 | 14:YE:308[B]:ALA:HB2 | 2.51 | 0.45 |
| 14:YE:73[F]:SER:HA | 14:YE:85[F]:THR:HA | 1.99 | 0.45 |
| 14:YF:135[C]:MET:SD | 14:YF:166[C]:PHE:HD1 | 2.40 | 0.45 |
| 14:YF:277[E]:VAL:HG11 | 14:YF:294[E]:GLU:HG2 | 1.98 | 0.45 |
| 14:YF:307[A]:TYR:HA | 14:YF:307[A]:TYR:HD1 | 1.66 | 0.45 |
| 11:BF:182:ASN:ND2 | 14:YF:327[E]:ASN:HD22 | 2.15 | 0.45 |
| 14:YF:10[A]:PRO:HD2 | 14:YF:349[A]:ASN:O | 2.16 | 0.45 |
| 14:YF:360[E]:ASN:N | 14:YF:360[E]:ASN:HD22 | 1.98 | 0.45 |
| 14:YF:20[E]:TYR:HA | 14:YF:69[E]:ILE:HD12 | 1.99 | 0.45 |
| 14:YF:73[B]:SER:HB2 | 14:YF:85[B]:THR:HG23 | 1.99 | 0.45 |
| 2:Z:479:TRP:CG | 2:Z:505:PRO:O | 2.69 | 0.45 |
| 2:Z:558:HIS:HB2 | 2:Z:569:VAL:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:50:GLY:HA2 | 2:Z:657:TYR:OH | 2.16 | 0.45 |
| 2:Z:761:GLU:HB2 | 2:Z:862:TYR:CZ | 2.51 | 0.45 |
| 15:ZA:66[D]:LYS:O | 15:ZA:68[D]:TYR:HD1 | 1.99 | 0.45 |
| 15:ZA:66[F]:LYS:O | 15:ZA:68[F]:TYR:HD1 | 1.99 | 0.45 |
| 4:AA:67:TYR:CE1 | 4:AA:84:ARG:HD3 | 2.52 | 0.45 |
| 4:AB:67:TYR:CE1 | 4:AB:84:ARG:HD3 | 2.52 | 0.45 |
| 5:AC:321:ALA:HA | 5:AC:358:VAL:CB | 2.44 | 0.45 |
| 5:AD:161:ASN:OD1 | 5:AD:249:ASP:HB3 | 2.15 | 0.45 |
| 5:AD:7:ILE:HD11 | 5:AE:24:ILE:HD11 | 1.99 | 0.45 |
| 5:AE:102:TRP:N | 5:AE:102:TRP:CD1 | 2.83 | 0.45 |
| 5:AE:103:ASN:CG | 5:AE:104:VAL:H | 2.20 | 0.45 |
| 5:AC:164:ARG:NH1 | 5:AE:192:ARG:HD3 | 2.32 | 0.45 |
| 6:AF:13:ARG:HG2 | 6:AF:14:LEU:N | 2.27 | 0.45 |
| 6:AH:126:VAL:HG12 | 6:AH:130:ARG:NH1 | 2.31 | 0.45 |
| 7:AJ:302:ILE:HD12 | 7:BA:306:PHE:CZ | 2.52 | 0.45 |
| 7:AJ:417:ASN:HB3 | 7:AJ:421:GLY:HA2 | 1.99 | 0.45 |
| 1:B:496:GLU:H | 1:B:496:GLU:HG2 | 1.57 | 0.45 |
| 7:BA:157:THR:OG1 | 7:BA:158:THR:N | 2.49 | 0.45 |
| 7:BA:36:ILE:O | 7:BA:39:ILE:HG13 | 2.17 | 0.45 |
| 8:BC:22:GLN:HE21 | 8:BC:33:THR:HG21 | 1.81 | 0.45 |
| 10:BE:287:VAL:O | 14:YE:100[C]:LYS:HD3 | 2.17 | 0.45 |
| 1:BH:113:THR:HA | 1:BH:162:PHE:HB3 | 1.99 | 0.45 |
| 1:BH:595:ILE:HG21 | 1:BH:602:ILE:HG23 | 1.99 | 0.45 |
| 2:BJ:479:TRP:CD1 | 2:BJ:505:PRO:O | 2.70 | 0.45 |
| 2:BJ:541:TYR:CG | 2:BJ:542:THR:N | 2.85 | 0.45 |
| 2:C:437:ASP:OD1 | 2:C:440:LEU:HB2 | 2.16 | 0.45 |
| 2:C:516:TRP:HE1 | 2:C:518:LYS:CG | 2.29 | 0.45 |
| 2:C:548:ILE:HG21 | 2:C:555:ARG:N | 2.32 | 0.45 |
| 3:CA:147:LEU:HD11 | 3:CA:152:GLU:CD | 2.37 | 0.45 |
| 3:CA:274:ILE:HD12 | 3:CA:311:TYR:HB3 | 1.99 | 0.45 |
| 3:CA:60:TYR:N | 3:CB:9:ARG:HH11 | 2.15 | 0.45 |
| 3:CB:106:PHE:CD2 | 3:CB:188:TRP:HH2 | 2.35 | 0.45 |
| 4:CD:1:MET:HG2 | 4:CD:70:HIS:ND1 | 2.32 | 0.45 |
| 4:CE:1:MET:HG2 | 4:CE:70:HIS:ND1 | 2.32 | 0.45 |
| 4:CE:68:GLN:HB3 | 4:CE:70:HIS:NE2 | 2.32 | 0.45 |
| 4:CE:67:TYR:CD1 | 4:CE:84:ARG:HB3 | 2.50 | 0.45 |
| 5:CF:133:LEU:HA | 5:CF:133:LEU:HD23 | 1.80 | 0.45 |
| 5:CF:20:ARG:NH1 | 5:CF:24:ILE:HD12 | 2.32 | 0.45 |
| 5:CF:317:LEU:HD13 | 5:CG:312:ARG:HH22 | 1.82 | 0.45 |
| 5:CG:359:GLU:O | 5:CG:370:HIS:N | 2.45 | 0.45 |
| 5:CG:469:PRO:HA | 5:CG:472:TYR:CZ | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:469:PRO:HA | 5:CH:472:TYR:CZ | 2.52 | 0.45 |
| 6:CI:126:VAL:HG12 | 6:CI:130:ARG:NH1 | 2.31 | 0.45 |
| 6:CJ:107:VAL:HG22 | 6:CJ:174:TYR:HD2 | 1.82 | 0.45 |
| 3:D:68:VAL:O | 3:D:71:MET:HB3 | 2.16 | 0.45 |
| 6:DA:172:SER:HA | 6:DA:176:ILE:O | 2.17 | 0.45 |
| 6:CI:13:ARG:NH1 | 6:DA:47:PHE:CE1 | 2.85 | 0.45 |
| 5:AC:348:THR:H | 7:DB:233:GLN:CG | 2.30 | 0.45 |
| 7:DC:165:THR:HA | 7:DC:168:LEU:HB2 | 1.99 | 0.45 |
| 7:DC:173:ILE:HD12 | 7:DC:176:ILE:HG21 | 1.98 | 0.45 |
| 7:DB:227:VAL:HG23 | 7:DC:225:LYS:HD3 | 1.99 | 0.45 |
| 7:DC:227:VAL:HG23 | 7:DD:225:LYS:HB3 | 1.98 | 0.45 |
| 7:DC:32:VAL:HG22 | 7:DC:36:ILE:HG12 | 1.99 | 0.45 |
| 7:DC:57:ILE:HG23 | 7:DD:56:GLY:CA | 2.46 | 0.45 |
| 7:AJ:71:ASN:CG | 7:DD:365:GLY:HA2 | 2.38 | 0.45 |
| 7:DB:95:TYR:HD1 | 7:DD:99:ARG:N | 2.15 | 0.45 |
| 8:DF:22:GLN:HE21 | 8:DF:33:THR:HG21 | 1.81 | 0.45 |
| 11:DI:32:TYR:HA | 11:DI:35:TYR:CD2 | 2.52 | 0.45 |
| 1:EA:568:ASN:OD1 | 1:EA:569:ILE:N | 2.50 | 0.45 |
| 1:EB:206:TRP:CE2 | 1:EB:222:THR:HB | 2.52 | 0.45 |
| 1:EB:583:SER:OG | 1:EB:584:ASP:N | 2.49 | 0.45 |
| 2:EC:220:LYS:HA | 5:EJ:562:SER:OG | 2.16 | 0.45 |
| 1:EA:60:LEU:HD13 | 2:EC:671:TYR:CD1 | 2.52 | 0.45 |
| 2:EC:865:LYS:HE3 | 2:EC:893:ILE:HD12 | 1.99 | 0.45 |
| 3:ED:197:ASP:OD1 | 3:ED:198:VAL:N | 2.45 | 0.45 |
| 3:ED:46:PRO:HA | 3:ED:270:ARG:CZ | 2.47 | 0.45 |
| 4:EG:68:GLN:HB3 | 4:EG:70:HIS:NE2 | 2.32 | 0.45 |
| 4:EG:67:TYR:CD1 | 4:EG:84:ARG:HB3 | 2.50 | 0.45 |
| 4:EG:113:ASN:ND2 | 4:EH:103:LEU:HD21 | 2.27 | 0.45 |
| 4:EG:240:VAL:HG22 | 4:EH:231:ILE:HD13 | 1.99 | 0.45 |
| 4:EF:15:ILE:HD13 | 4:EH:25:PHE:HB2 | 1.99 | 0.45 |
| 5:EI:103:ASN:O | 5:EI:104:VAL:C | 2.56 | 0.45 |
| 5:EJ:443:PHE:O | 5:FA:408:VAL:HG13 | 2.16 | 0.45 |
| 5:EI:572:ALA:HA | 5:EJ:540:GLU:HG2 | 1.98 | 0.45 |
| 2:EC:221:ALA:O | 5:EJ:564:PRO:HG2 | 2.17 | 0.45 |
| 5:EJ:80:ASN:C | 5:EJ:81:LEU:HD12 | 2.38 | 0.45 |
| 4:F:67:TYR:CE1 | 4:F:84:ARG:HD3 | 2.52 | 0.45 |
| 6:FD:107:VAL:HG22 | 6:FD:174:TYR:HD2 | 1.82 | 0.45 |
| 7:FE:231:GLY:H | 7:FE:243:VAL:HB | 1.81 | 0.45 |
| 7:FE:415:ASN:O | 7:FE:424:ARG:HD2 | 2.17 | 0.45 |
| 7:FF:111:ASN:ND2 | 7:FF:114:SER:HB3 | 2.32 | 0.45 |
| 7:FE:265:LEU:N | 7:FF:256:THR:O | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FG:101:SER:OG | 7:FG:105:GLU:HB2 | 2.17 | 0.45 |
| 4:G:205:THR:OG1 | 4:H:199:MET:SD | 2.75 | 0.45 |
| 12:GC:120:SER:HA | 12:GC:123:LEU:HG | 1.97 | 0.45 |
| 1:GD:328:LEU:HD23 | 1:GD:328:LEU:HA | 1.71 | 0.45 |
| 1:GE:349:VAL:HG13 | 1:GE:392:ILE:HD11 | 1.98 | 0.45 |
| 2:GF:202:PHE:HB3 | 2:GF:209:VAL:HG22 | 1.98 | 0.45 |
| 2:GF:29:GLY:HA2 | 3:GH:60:TYR:HB3 | 1.99 | 0.45 |
| 2:GF:479:TRP:CD1 | 2:GF:505:PRO:O | 2.70 | 0.45 |
| 2:GF:549:PRO:HB2 | 2:GF:550:GLU:OE1 | 2.17 | 0.45 |
| 2:GF:81:ARG:HD3 | 2:GF:96:TYR:CE1 | 2.51 | 0.45 |
| 2:GF:921:TRP:CD1 | 2:GF:921:TRP:N | 2.85 | 0.45 |
| 3:GH:199:SER:OG | 3:GH:200:ILE:N | 2.50 | 0.45 |
| 3:GH:76:MET:O | 3:GH:299:PRO:HD3 | 2.16 | 0.45 |
| 4:GI:67:TYR:CE1 | 4:GI:84:ARG:HD3 | 2.52 | 0.45 |
| 4:HA:67:TYR:CE1 | 4:HA:84:ARG:HD3 | 2.52 | 0.45 |
| 5:HB:103:ASN:O | 5:HB:104:VAL:C | 2.56 | 0.45 |
| 5:HB:213:GLY:CA | 5:HB:221:GLU:HB2 | 2.47 | 0.45 |
| 5:HB:290:SER:N | 5:HB:371:PHE:O | 2.49 | 0.45 |
| 5:HC:302:GLU:HB3 | 5:HC:365:ILE:CD1 | 2.47 | 0.45 |
| 5:HD:157:SER:O | 5:HD:160:SER:OG | 2.28 | 0.45 |
| 5:HC:255:ARG:HH21 | 5:HD:249:ASP:HB2 | 1.82 | 0.45 |
| 5:HD:340:VAL:HG22 | 6:HE:173:THR:HA | 1.98 | 0.45 |
| 6:HE:172:SER:HA | 6:HE:176:ILE:O | 2.17 | 0.45 |
| 6:HF:172:SER:HA | 6:HF:176:ILE:O | 2.17 | 0.45 |
| 6:HF:32:ARG:NH1 | 6:HG:144:ASN:OD1 | 2.47 | 0.45 |
| 6:HG:172:SER:HA | 6:HG:176:ILE:O | 2.17 | 0.45 |
| 7:HH:462:ASN:HB3 | 7:HJ:482:TYR:HD1 | 1.82 | 0.45 |
| 7:HH:161:THR:HA | 7:HI:158:THR:O | 2.17 | 0.45 |
| 7:HI:368:SER:HA | 7:HI:389:ASN:ND2 | 2.32 | 0.45 |
| 5:I:184:THR:H | 5:I:307:ASN:ND2 | 2.13 | 0.45 |
| 5:I:213:GLY:CA | 5:I:221:GLU:HB2 | 2.47 | 0.45 |
| 5:I:322:GLY:HA2 | 5:I:360:THR:H | 1.81 | 0.45 |
| 8:FH:41:LEU:HD22 | 8:IA:140:LEU:HD23 | 1.99 | 0.45 |
| 8:IB:114:ARG:HD2 | 8:IB:123:VAL:HG11 | 1.98 | 0.45 |
| 11:IE:32:TYR:HA | 11:IE:35:TYR:CD2 | 2.52 | 0.45 |
| 5:J:323:THR:HB | 5:J:355:ASP:HB3 | 1.99 | 0.45 |
| 5:J:49:TRP:CZ3 | 5:J:96:ARG:HD2 | 2.52 | 0.45 |
| 6:N:172:SER:HA | 6:N:176:ILE:O | 2.17 | 0.45 |
| 7:O:288:ILE:O | 7:P:288:ILE:N | 2.44 | 0.45 |
| 7:Q:359:TRP:CZ2 | 7:Q:524:LYS:HD3 | 2.52 | 0.45 |
| 11:V:5:PHE:CE2 | 11:V:188:MET:HG2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:V:30:ARG:NH1 | 11:V:192:TYR:HD1 | 2.14 | 0.45 |
| 1:X:81:ARG:HA | 1:X:326:ARG:HG3 | 1.99 | 0.45 |
| 1:Y:374:ILE:HB | 1:Y:408:ILE:HG12 | 1.98 | 0.45 |
| 1:Y:647:ARG:HD3 | 1:Y:650:TYR:CE2 | 2.50 | 0.45 |
| 13:YA:146[E]:VAL:O | 13:YA:150[E]:SER:OG | 2.34 | 0.45 |
| 13:YA:261[B]:LYS:HE2 | 13:YA:293[B]:ASN:HB3 | 1.99 | 0.45 |
| 13:YA:266[D]:TRP:CD1 | 13:YA:274[D]:GLN:HG2 | 2.52 | 0.45 |
| 13:YA:261[D]:LYS:HE2 | 13:YA:293[D]:ASN:HB3 | 1.99 | 0.45 |
| 13:YA:314[B]:SER:OG | 13:YA:316[B]:TRP:HB3 | 2.17 | 0.45 |
| 13:YA:478[E]:ASN:N | 13:YC:485[E]:ASP:O | 2.49 | 0.45 |
| 13:YA:521[C]:LEU:HD12 | 13:YA:522[C]:VAL:N | 2.32 | 0.45 |
| 13:YA:521[B]:LEU:HD12 | 13:YA:522[B]:VAL:N | 2.32 | 0.45 |
| 13:YA:521[F]:LEU:HD12 | 13:YA:522[F]:VAL:N | 2.32 | 0.45 |
| 13:YA:537[E]:LYS:HD3 | 13:YA:537[E]:LYS:C | 2.37 | 0.45 |
| 13:YB:146[C]:VAL:O | 13:YB:150[C]:SER:OG | 2.34 | 0.45 |
| 13:YB:314[E]:SER:OG | 13:YB:316[E]:TRP:HB3 | 2.17 | 0.45 |
| 13:YB:314[D]:SER:OG | 13:YB:316[D]:TRP:HB3 | 2.17 | 0.45 |
| 13:YB:460[A]:GLY:HA3 | 13:YC:453[A]:ASP:HA | 1.98 | 0.45 |
| 13:YB:552[A]:GLU:HB2 | 13:YC:544[A]:TRP:HB2 | 1.98 | 0.45 |
| 13:YB:552[D]:GLU:HB2 | 13:YC:544[D]:TRP:HB2 | 1.98 | 0.45 |
| 13:YB:553[D]:LYS:HB2 | 13:YB:553[D]:LYS:HZ2 | 1.81 | 0.45 |
| 13:YB:67[E]:SER:HB3 | 13:YC:123[E]:ARG:HB2 | 1.98 | 0.45 |
| 13:YB:67[B]:SER:HB3 | 13:YC:123[B]:ARG:HB2 | 1.99 | 0.45 |
| 13:YC:261[E]:LYS:HE2 | 13:YC:293[E]:ASN:HB3 | 1.99 | 0.45 |
| 13:YC:314[B]:SER:OG | 13:YC:316[B]:TRP:HB3 | 2.17 | 0.45 |
| 13:YC:315[B]:LEU:O | 13:YC:319[B]:GLN:HG2 | 2.16 | 0.45 |
| 13:YB:70[A]:GLY:O | 13:YC:394[A]:GLU:N | 2.50 | 0.45 |
| 13:YC:521[B]:LEU:HD12 | 13:YC:522[B]:VAL:N | 2.32 | 0.45 |
| 13:YA:47[F]:ILE:HG12 | 14:YD:123[F]:PRO:HD3 | 1.99 | 0.45 |
| 14:YD:160[D]:ILE:HG21 | 14:YD:282[D]:ALA:HB1 | 1.97 | 0.45 |
| 14:YD:135[A]:MET:SD | 14:YD:166[A]:PHE:HD1 | 2.40 | 0.45 |
| 14:YD:266[E]:ILE:HD11 | 14:YD:290[E]:ASN:CG | 2.37 | 0.45 |
| 14:YD:307[D]:TYR:HD1 | 14:YD:307[D]:TYR:HA | 1.66 | 0.45 |
| 14:YD:307[E]:TYR:HD1 | 14:YD:307[E]:TYR:HA | 1.66 | 0.45 |
| 14:YD:73[E]:SER:HB2 | 14:YD:85[E]:THR:HG23 | 1.99 | 0.45 |
| 14:YD:73[A]:SER:HA | 14:YD:85[A]:THR:HA | 1.99 | 0.45 |
| 14:YD:73[B]:SER:HA | 14:YD:85[B]:THR:HA | 1.99 | 0.45 |
| 14:YE:135[E]:MET:SD | 14:YE:166[E]:PHE:HD1 | 2.40 | 0.45 |
| 14:YE:236[E]:TRP:CD1 | 14:YE:308[E]:ALA:HB2 | 2.51 | 0.45 |
| 14:YF:140[D]:TYR:HE2 | 14:YF:148[D]:PRO:HD3 | 1.82 | 0.45 |
| 14:YF:279[F]:ARG:HA | 14:YF:279[F]:ARG:HD3 | 1.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:277[C]:VAL:HG11 | 14:YF:294[C]:GLU:HG2 | 1.99 | 0.45 |
| 2:Z:479:TRP:HE3 | 2:Z:479:TRP:H | 1.64 | 0.45 |
| 2:Z:965:LEU:HG | 2:Z:982:LEU:HD11 | 1.99 | 0.45 |
| 4:AA:22:ASP:O | 4:AA:26:ASP:N | 2.26 | 0.45 |
| 5:AC:290:SER:N | 5:AC:371:PHE:O | 2.49 | 0.45 |
| 5:AC:60:LEU:CG | 5:AC:79:ILE:HG22 | 2.46 | 0.45 |
| 5:AD:190:ASN:HD22 | 5:AD:247:PHE:HD2 | 1.64 | 0.45 |
| 5:AD:469:PRO:HA | 5:AD:472:TYR:CZ | 2.52 | 0.45 |
| 5:AE:310:GLU:HB2 | 5:AE:384:THR:HB | 1.98 | 0.45 |
| 5:AE:469:PRO:HA | 5:AE:472:TYR:CZ | 2.52 | 0.45 |
| 6:AF:172:SER:HA | 6:AF:176:ILE:O | 2.17 | 0.45 |
| 6:AF:213:TYR:OH | 7:DC:171:LYS:HG3 | 2.17 | 0.45 |
| 6:AG:13:ARG:HG2 | 6:AG:14:LEU:N | 2.27 | 0.45 |
| 7:AJ:110:VAL:HG12 | 7:AJ:111:ASN:N | 2.32 | 0.45 |
| 1:B:470:ASP:O | 1:B:472:ASP:N | 2.50 | 0.45 |
| 7:AI:462:ASN:HB3 | 7:BA:482:TYR:HD1 | 1.82 | 0.45 |
| 10:BE:221:ALA:O | 10:BE:224:ASN:HB3 | 2.16 | 0.45 |
| 10:BE:237:THR:HA | 10:BE:287:VAL:CG2 | 2.47 | 0.45 |
| 11:BF:88:THR:HG22 | 11:BF:92:ALA:HB3 | 1.99 | 0.45 |
| 2:BJ:654:PRO:HG3 | 9:DG:47:ARG:CD | 2.47 | 0.45 |
| 2:BJ:911:THR:HG23 | 3:CA:330:ILE:HG12 | 1.99 | 0.45 |
| 2:C:380:ILE:O | 2:C:401:LYS:HA | 2.17 | 0.45 |
| 3:CA:87:ASP:OD2 | 3:CA:202:ARG:HD2 | 2.17 | 0.45 |
| 3:CB:40:THR:OG1 | 3:CB:273:SER:HB3 | 2.17 | 0.45 |
| 4:CC:1:MET:HG2 | 4:CC:70:HIS:ND1 | 2.32 | 0.45 |
| 5:CF:275:SER:HA | 5:CF:280:ILE:HG22 | 1.99 | 0.45 |
| 5:CF:293:PHE:HA | 5:CF:295:ALA:H | 1.82 | 0.45 |
| 5:CF:321:ALA:HA | 5:CF:358:VAL:CB | 2.44 | 0.45 |
| 5:CF:90:ASN:HD21 | 5:CG:49:TRP:C | 2.18 | 0.45 |
| 5:CG:161:ASN:OD1 | 5:CG:249:ASP:HB3 | 2.16 | 0.45 |
| 5:CF:386:PHE:CZ | 5:CG:390:LEU:HD13 | 2.52 | 0.45 |
| 5:CG:466:PRO:HA | 5:CG:596:TYR:CZ | 2.52 | 0.45 |
| 5:CH:176:ASP:HA | 5:CH:231:ARG:HA | 1.99 | 0.45 |
| 5:CH:69:ALA:HB1 | 5:CH:98:VAL:HG23 | 1.99 | 0.45 |
| 6:CJ:144:ASN:HB3 | 6:CJ:159:THR:HG22 | 1.99 | 0.45 |
| 6:DA:144:ASN:HB3 | 6:DA:159:THR:HG22 | 1.99 | 0.45 |
| 7:DB:382:ARG:HH22 | 7:DB:434:VAL:HB | 1.81 | 0.45 |
| 7:DB:39:ILE:HD13 | 7:DD:39:ILE:HD13 | 1.99 | 0.45 |
| 7:DB:190:VAL:HB | 7:DC:188:GLN:C | 2.36 | 0.45 |
| 7:DC:77:THR:HA | 7:DD:74:LYS:O | 2.17 | 0.45 |
| 7:DD:407:SER:HA | 7:DD:410:THR:OG1 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:DE:22:GLN:HE21 | 8:DE:33:THR:HG21 | 1.81 | 0.45 |
| 3:E:24:PHE:O | 3:E:28:ILE:HD12 | 2.16 | 0.45 |
| 1:EA:236:PHE:N | 1:EA:236:PHE:CD1 | 2.84 | 0.45 |
| 1:EA:7:ASN:N | 1:EA:7:ASN:OD1 | 2.50 | 0.45 |
| 1:EB:40:GLN:HE21 | 1:EB:43:PHE:HB2 | 1.81 | 0.45 |
| 2:EC:336:ILE:HG21 | 2:EC:350:PHE:O | 2.17 | 0.45 |
| 2:EC:548:ILE:HG21 | 2:EC:555:ARG:N | 2.32 | 0.45 |
| 2:EC:37:GLU:O | 2:EC:80:ILE:HA | 2.17 | 0.45 |
| 3:ED:147:LEU:HD11 | 3:ED:152:GLU:CD | 2.37 | 0.45 |
| 3:ED:68:VAL:O | 3:ED:71:MET:HB3 | 2.17 | 0.45 |
| 4:EF:32:ASN:HD21 | 4:EG:10:ILE:HB | 1.82 | 0.45 |
| 4:EH:111:ASN:HB2 | 4:EH:116:ILE:HD12 | 1.98 | 0.45 |
| 4:EH:1:MET:HG2 | 4:EH:70:HIS:ND1 | 2.32 | 0.45 |
| 5:EI:23:GLY:O | 5:EI:24:ILE:HB | 2.15 | 0.45 |
| 5:EI:54:ALA:HB2 | 5:EI:71:ASN:O | 2.16 | 0.45 |
| 5:EJ:363:ASN:N | 5:EJ:367:GLU:OE2 | 2.49 | 0.45 |
| 2:EC:228:ARG:NH2 | 5:FA:559:PRO:HB3 | 2.25 | 0.45 |
| 5:FA:563:GLY:N | 5:FA:564:PRO:HD3 | 2.31 | 0.45 |
| 5:FA:71:ASN:OD1 | 5:FA:73:SER:N | 2.32 | 0.45 |
| 6:FC:135:GLU:O | 6:FC:139:SER:N | 2.26 | 0.45 |
| 6:FC:107:VAL:HG22 | 6:FC:174:TYR:HD2 | 1.82 | 0.45 |
| 6:FD:195:LEU:HD13 | 6:FD:215:PHE:CE1 | 2.52 | 0.45 |
| 7:FE:32:VAL:O | 7:FE:36:ILE:N | 2.39 | 0.45 |
| 7:FE:349:TRP:NE1 | 7:FE:353:SER:O | 2.50 | 0.45 |
| 7:FE:405:ARG:NH2 | 7:FE:409:LEU:O | 2.49 | 0.45 |
| 7:FE:444:TYR:HB2 | 7:FG:486:ASP:HB2 | 1.99 | 0.45 |
| 6:CJ:205:ASN:HB2 | 7:FF:175:GLN:O | 2.17 | 0.45 |
| 7:FE:188:GLN:NE2 | 7:FG:192:GLN:OE1 | 2.50 | 0.45 |
| 7:FE:346:ILE:N | 7:FG:348:MET:O | 2.27 | 0.45 |
| 5:EJ:196:ARG:NE | 7:FG:5:THR:HG23 | 2.32 | 0.45 |
| 8:R:99:ILE:HD11 | 8:FH:55:ASN:HD22 | 1.80 | 0.45 |
| 8:FH:98:GLU:OE1 | 8:FH:98:GLU:N | 2.48 | 0.45 |
| 12:GC:22:PHE:CG | 12:IF:228:LEU:HD13 | 2.52 | 0.45 |
| 1:GD:113:THR:HA | 1:GD:162:PHE:HB3 | 1.99 | 0.45 |
| 1:GD:642:PHE:HE1 | 1:GD:651:LEU:HD13 | 1.82 | 0.45 |
| 2:GF:168:ILE:HA | 2:GF:168:ILE:HD12 | 1.88 | 0.45 |
| 2:GF:336:ILE:HG21 | 2:GF:350:PHE:O | 2.17 | 0.45 |
| 2:GF:546:GLU:OE1 | 2:GF:546:GLU:N | 2.49 | 0.45 |
| 2:GF:548:ILE:HG21 | 2:GF:555:ARG:N | 2.32 | 0.45 |
| 2:GF:796:THR:HG23 | 2:GF:797:TYR:CD2 | 2.52 | 0.45 |
| 2:GF:865:LYS:HE3 | 2:GF:893:ILE:HD12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:67:TYR:CE1 | 4:H:84:ARG:HD3 | 2.52 | 0.45 |
| 5:HB:361:ASP:N | 5:HB:365:ILE:O | 2.50 | 0.45 |
| 5:HC:443:PHE:O | 5:HD:408:VAL:HG13 | 2.16 | 0.45 |
| 5:HD:265:LEU:HB3 | 5:HD:281:TYR:HB3 | 1.99 | 0.45 |
| 7:HH:65:GLU:O | 7:HH:69:GLY:N | 2.48 | 0.45 |
| 7:HI:302:ILE:HD12 | 7:HJ:306:PHE:CZ | 2.52 | 0.45 |
| 5:I:20:ARG:NH1 | 5:I:24:ILE:HD12 | 2.32 | 0.45 |
| 8:IA:114:ARG:HD2 | 8:IA:123:VAL:HG11 | 1.97 | 0.45 |
| 8:IB:135:THR:HG22 | 8:IB:156:THR:O | 2.16 | 0.45 |
| 12:GC:14:ALA:O | 12:IF:166:SER:HB2 | 2.16 | 0.45 |
| 5:J:126:ILE:HD12 | 5:J:133:LEU:HD11 | 1.98 | 0.45 |
| 5:K:199:GLU:HG3 | 5:K:200:LEU:N | 2.32 | 0.45 |
| 6:L:107:VAL:HG22 | 6:L:174:TYR:HD2 | 1.82 | 0.45 |
| 6:L:135:GLU:O | 6:L:139:SER:N | 2.26 | 0.45 |
| 6:L:203:LEU:HD12 | 6:L:206:GLN:NE2 | 2.31 | 0.45 |
| 7:O:283:TRP:CZ3 | 7:O:284:ASN:HB3 | 2.52 | 0.45 |
| 7:O:346:ILE:HD11 | 7:Q:350:ALA:HB2 | 1.99 | 0.45 |
| 7:O:39:ILE:HD13 | 7:Q:39:ILE:HD13 | 1.99 | 0.45 |
| 7:P:172:LEU:O | 7:P:175:GLN:NE2 | 2.49 | 0.45 |
| 7:P:29:ILE:O | 7:P:30:THR:OG1 | 2.24 | 0.45 |
| 7:P:302:ILE:HD12 | 7:Q:306:PHE:CZ | 2.52 | 0.45 |
| 7:P:417:ASN:HB3 | 7:P:421:GLY:HA2 | 1.99 | 0.45 |
| 7:Q:413:ASN:O | 7:Q:424:ARG:HD3 | 2.17 | 0.45 |
| 8:R:6:VAL:HB | 8:S:53:PHE:CD1 | 2.51 | 0.45 |
| 12:W:166:SER:HB2 | 12:IF:14:ALA:O | 2.17 | 0.45 |
| 12:W:195:VAL:O | 12:W:195:VAL:HG12 | 2.16 | 0.45 |
| 1:Y:491:PHE:HE2 | 1:Y:619:GLN:HA | 1.82 | 0.45 |
| 1:Y:90:VAL:O | 1:Y:94:GLN:HG2 | 2.17 | 0.45 |
| 13:YA:121[A]:TYR:OH | 13:YA:123[A]:ARG:NH2 | 2.50 | 0.45 |
| 13:YA:304[E]:TRP:O | 13:YA:308[E]:TYR:N | 2.33 | 0.45 |
| 13:YA:314[A]:SER:OG | 13:YA:316[A]:TRP:HB3 | 2.17 | 0.45 |
| 13:YA:452[D]:GLY:O | 13:YC:460[D]:GLY:N | 2.51 | 0.45 |
| 13:YA:490[F]:VAL:HG12 | 13:YA:492[F]:GLY:H | 1.81 | 0.45 |
| 13:YA:543[A]:ASP:HA | 13:YC:551[A]:THR:O | 2.17 | 0.45 |
| 13:YA:558[A]:SER:N | 13:YB:550[A]:TRP:O | 2.50 | 0.45 |
| 13:YA:61[D]:ILE:HA | 13:YB:76[D]:PRO:HA | 1.96 | 0.45 |
| 13:YB:110[E]:ARG:HD2 | 13:YB:118[E]:THR:O | 2.17 | 0.45 |
| 13:YB:236[F]:ILE:HG23 | 13:YB:240[F]:GLU:HB2 | 1.99 | 0.45 |
| 13:YB:314[F]:SER:OG | 13:YB:316[F]:TRP:HB3 | 2.17 | 0.45 |
| 13:YB:416[F]:HIS:CG | 13:YB:417[F]:PRO:HD2 | 2.51 | 0.45 |
| 13:YB:76[C]:PRO:HB2 | 13:YB:98[C]:GLY:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:7[E]:ASN:ND2 | 13:YB:9[E]:ASN:HA | 2.21 | 0.45 |
| 13:YC:146[F]:VAL:O | 13:YC:150[F]:SER:OG | 2.34 | 0.45 |
| 13:YC:296[F]:LEU:HA | 13:YC:296[F]:LEU:HD12 | 1.84 | 0.45 |
| 13:YC:314[D]:SER:OG | 13:YC:316[D]:TRP:HB3 | 2.17 | 0.45 |
| 13:YA:452[A]:GLY:CA | 13:YC:321[A]:LYS:HD3 | 2.40 | 0.45 |
| 13:YC:416[D]:HIS:CG | 13:YC:417[D]:PRO:HD2 | 2.51 | 0.45 |
| 13:YB:458[E]:VAL:HG21 | 13:YC:454[E]:LYS:HD2 | 1.99 | 0.45 |
| 13:YC:76[B]:PRO:HB2 | 13:YC:98[B]:GLY:C | 2.37 | 0.45 |
| 14:YD:140[B]:TYR:HE2 | 14:YD:148[B]:PRO:HD3 | 1.82 | 0.45 |
| 14:YD:242[B]:PRO:HD2 | 14:YE:91[B]:LYS:O | 2.17 | 0.45 |
| 14:YD:242[D]:PRO:HD2 | 14:YE:91[D]:LYS:O | 2.17 | 0.45 |
| 14:YD:288[E]:TYR:CE1 | 14:YD:371[E]:LYS:HD3 | 2.52 | 0.45 |
| 14:YD:360[C]:ASN:N | 14:YD:360[C]:ASN:HD22 | 1.97 | 0.45 |
| 14:YD:73[B]:SER:HB2 | 14:YD:85[B]:THR:HG23 | 1.99 | 0.45 |
| 10:GA:287:VAL:O | 14:YE:100[E]:LYS:HD3 | 2.17 | 0.45 |
| 14:YE:10[C]:PRO:HD2 | 14:YE:349[C]:ASN:O | 2.17 | 0.45 |
| 14:YE:234[B]:PHE:HD1 | 14:YF:97[B]:VAL:HG12 | 1.82 | 0.45 |
| 14:YE:73[A]:SER:HA | 14:YE:85[A]:THR:HA | 1.99 | 0.45 |
| 14:YF:160[F]:ILE:HG21 | 14:YF:282[F]:ALA:HB1 | 1.98 | 0.45 |
| 14:YF:178[C]:LEU:CD1 | 14:YF:183[C]:ASP:HA | 2.46 | 0.45 |
| 14:YF:236[F]:TRP:CD1 | 14:YF:308[F]:ALA:HB2 | 2.51 | 0.45 |
| 14:YF:266[C]:ILE:HD11 | 14:YF:290[C]:ASN:CG | 2.37 | 0.45 |
| 14:YF:279[A]:ARG:HD3 | 14:YF:279[A]:ARG:HA | 1.43 | 0.45 |
| 14:YF:10[B]:PRO:HD2 | 14:YF:349[B]:ASN:O | 2.17 | 0.45 |
| 14:YF:73[E]:SER:HB2 | 14:YF:85[E]:THR:HG23 | 1.99 | 0.45 |
| 14:YE:236[C]:TRP:N | 14:YF:95[C]:VAL:O | 2.50 | 0.45 |
| 2:Z:380:ILE:O | 2:Z:401:LYS:HA | 2.17 | 0.45 |
| 2:Z:425:ARG:NH2 | 2:Z:447:ASN:HD21 | 2.15 | 0.45 |
| 2:Z:479:TRP:CD1 | 2:Z:505:PRO:O | 2.70 | 0.45 |
| 2:Z:37:GLU:O | 2:Z:80:ILE:HA | 2.17 | 0.45 |
| 1:A:568:ASN:OD1 | 1:A:569:ILE:N | 2.49 | 0.44 |
| 4:AB:67:TYR:CD1 | 4:AB:84:ARG:HB3 | 2.50 | 0.44 |
| 5:AC:322:GLY:HA2 | 5:AC:360:THR:H | 1.81 | 0.44 |
| 5:AD:249:ASP:CA | 5:AE:158:ASP:HB3 | 2.47 | 0.44 |
| 5:AE:304:ILE:HD11 | 5:AE:366:PRO:HG3 | 1.99 | 0.44 |
| 5:AE:69:ALA:HB1 | 5:AE:98:VAL:HG23 | 1.99 | 0.44 |
| 6:AG:172:SER:HA | 6:AG:176:ILE:O | 2.17 | 0.44 |
| 7:AI:382:ARG:HG3 | 7:AI:383:TYR:CD2 | 2.52 | 0.44 |
| 7:AI:519:LEU:HA | 7:AJ:434:VAL:HG13 | 1.99 | 0.44 |
| 7:AI:190:VAL:HG23 | 7:AJ:188:GLN:HB3 | 1.99 | 0.44 |
| 7:AJ:57:ILE:HG23 | 7:BA:56:GLY:CA | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:506:LYS:O | 1:B:509:SER:OG | 2.19 | 0.44 |
| 11:BF:32:TYR:HA | 11:BF:35:TYR:CD2 | 2.52 | 0.44 |
| 1:BH:106:ALA:HB3 | 1:BH:169:GLN:HB2 | 1.98 | 0.44 |
| 1:BH:12:ARG:O | 2:BJ:709:TYR:OH | 2.24 | 0.44 |
| 1:BH:288:TYR:CE2 | 1:BH:290:ASP:O | 2.70 | 0.44 |
| 1:BI:332:LYS:O | 1:BI:335:THR:HG22 | 2.18 | 0.44 |
| 1:BI:472:ASP:OD2 | 1:BI:474:SER:HB2 | 2.17 | 0.44 |
| 2:BJ:202:PHE:HB3 | 2:BJ:209:VAL:HG22 | 1.98 | 0.44 |
| 2:BJ:209:VAL:O | 2:BJ:221:ALA:HA | 2.16 | 0.44 |
| 2:BJ:548:ILE:HG21 | 2:BJ:555:ARG:N | 2.32 | 0.44 |
| 2:BJ:543:LYS:HG2 | 2:BJ:575:PHE:CE1 | 2.52 | 0.44 |
| 2:BJ:965:LEU:HG | 2:BJ:982:LEU:HD11 | 1.99 | 0.44 |
| 2:BJ:975:ASN:OD1 | 2:BJ:981:GLN:HB3 | 2.16 | 0.44 |
| 2:BJ:982:LEU:O | 2:BJ:982:LEU:HD12 | 2.17 | 0.44 |
| 2:C:191:TYR:HE2 | 2:C:204:ARG:HB3 | 1.82 | 0.44 |
| 2:C:711:ARG:HD3 | 2:C:878:ASP:OD1 | 2.18 | 0.44 |
| 2:C:819:ARG:O | 2:C:820:LEU:HD23 | 2.17 | 0.44 |
| 3:CB:197:ASP:OD1 | 3:CB:198:VAL:N | 2.48 | 0.44 |
| 4:CE:111:ASN:HB2 | 4:CE:116:ILE:HD12 | 1.98 | 0.44 |
| 4:CD:173:SER:N | 4:CE:166:SER:OG | 2.40 | 0.44 |
| 5:CF:139:ALA:O | 5:CF:141:GLY:N | 2.47 | 0.44 |
| 5:CF:290:SER:CA | 5:CF:371:PHE:H | 2.30 | 0.44 |
| 5:CF:361:ASP:N | 5:CF:365:ILE:O | 2.50 | 0.44 |
| 5:CG:146:VAL:HG11 | 5:CH:151:ILE:O | 2.16 | 0.44 |
| 5:CG:206:PHE:HB3 | 5:CG:223:VAL:HG13 | 1.99 | 0.44 |
| 5:CG:323:THR:HB | 5:CG:355:ASP:HB3 | 1.99 | 0.44 |
| 5:CG:363:ASN:N | 5:CG:367:GLU:OE2 | 2.49 | 0.44 |
| 5:CH:131:SER:HA | 5:CH:150:GLN:HA | 1.99 | 0.44 |
| 5:CH:310:GLU:HB2 | 5:CH:384:THR:HB | 1.98 | 0.44 |
| 5:CF:394:LEU:HD22 | 5:CH:395:THR:HA | 1.99 | 0.44 |
| 3:D:87:ASP:OD2 | 3:D:202:ARG:HD2 | 2.17 | 0.44 |
| 3:D:47:TRP:HZ3 | 3:D:270:ARG:HD3 | 1.79 | 0.44 |
| 6:CI:10:VAL:CG1 | 6:DA:10:VAL:HG21 | 2.47 | 0.44 |
| 7:DB:329:ASN:OD1 | 7:DB:330:ARG:N | 2.50 | 0.44 |
| 7:DB:382:ARG:HG3 | 7:DB:383:TYR:CD2 | 2.52 | 0.44 |
| 7:DC:59:PHE:CZ | 7:DD:55:LYS:HG3 | 2.52 | 0.44 |
| 7:DD:335:ASN:OD1 | 7:DD:336:GLU:N | 2.47 | 0.44 |
| 8:DE:53:PHE:HB2 | 12:DJ:7:PHE:CE2 | 2.52 | 0.44 |
| 8:BC:41:LEU:HD22 | 8:DF:140:LEU:HD23 | 1.98 | 0.44 |
| 8:DE:6:VAL:HB | 8:DF:53:PHE:CD1 | 2.52 | 0.44 |
| 12:DJ:99:SER:HB3 | 12:DJ:102:GLY:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:196:PRO:O | 3:E:199:SER:OG | 2.25 | 0.44 |
| 1:EA:116:ASP:OD1 | 1:EA:118:LEU:N | 2.46 | 0.44 |
| 1:EA:345:TYR:OH | 1:EA:400:ASN:ND2 | 2.51 | 0.44 |
| 1:EA:69:GLN:CD | 1:EB:21:PHE:HZ | 2.20 | 0.44 |
| 1:EB:188:TYR:HD1 | 1:EB:233:ASN:ND2 | 2.15 | 0.44 |
| 2:EC:400:ASP:O | 2:EC:424:ARG:NH1 | 2.50 | 0.44 |
| 2:EC:369:ASP:HB2 | 2:EC:434:MET:HG2 | 1.99 | 0.44 |
| 2:EC:724:ALA:O | 2:EC:725:ARG:HG2 | 2.17 | 0.44 |
| 2:EC:796:THR:HG23 | 2:EC:797:TYR:CD2 | 2.52 | 0.44 |
| 2:EC:819:ARG:O | 2:EC:820:LEU:HD23 | 2.17 | 0.44 |
| 3:ED:201:ASN:OD1 | 5:EI:10:VAL:HG21 | 2.17 | 0.44 |
| 3:ED:249:PHE:O | 3:ED:329:ASN:HA | 2.16 | 0.44 |
| 4:EF:152:SER:O | 4:EF:158:SER:HA | 2.18 | 0.44 |
| 4:EH:79:VAL:N | 4:EH:97:ILE:O | 2.32 | 0.44 |
| 5:EI:248:MET:HB2 | 5:EI:254:TRP:CD1 | 2.52 | 0.44 |
| 5:EI:321:ALA:HA | 5:EI:358:VAL:CB | 2.44 | 0.44 |
| 5:EJ:206:PHE:HB3 | 5:EJ:223:VAL:HG13 | 1.99 | 0.44 |
| 5:EJ:302:GLU:HB3 | 5:EJ:365:ILE:CD1 | 2.47 | 0.44 |
| 5:FA:22:GLY:O | 5:FA:26:ILE:HG22 | 2.16 | 0.44 |
| 5:FA:69:ALA:HB1 | 5:FA:98:VAL:HG23 | 1.99 | 0.44 |
| 6:FB:117:THR:H | 6:FB:120:MET:HE3 | 1.82 | 0.44 |
| 6:FC:108:LEU:HD23 | 6:FC:113:PRO:HA | 2.00 | 0.44 |
| 7:FE:323:GLY:HA2 | 7:FF:326:ILE:HG23 | 1.98 | 0.44 |
| 7:FF:110:VAL:HG12 | 7:FF:111:ASN:N | 2.32 | 0.44 |
| 7:FF:116:ILE:HG23 | 7:FF:120:LYS:HB2 | 2.00 | 0.44 |
| 7:FF:118:PRO:HB3 | 7:FG:106:ALA:O | 2.17 | 0.44 |
| 7:FF:117:THR:HG22 | 7:FF:120:LYS:NZ | 2.32 | 0.44 |
| 7:FE:347:MET:HE2 | 7:FF:345:ALA:HB1 | 1.99 | 0.44 |
| 7:FE:476:ASP:N | 7:FF:470:GLY:O | 2.38 | 0.44 |
| 7:FG:100:TYR:CE1 | 7:FG:115:SER:HB2 | 2.52 | 0.44 |
| 9:FJ:33:LYS:HG2 | 9:FJ:122:ILE:HG21 | 1.99 | 0.44 |
| 4:F:168:PHE:CE1 | 4:G:149:ARG:HB3 | 2.52 | 0.44 |
| 10:GA:37:GLN:HB3 | 10:GA:128:LEU:HB3 | 1.99 | 0.44 |
| 11:GB:5:PHE:CE2 | 11:GB:188:MET:HG2 | 2.52 | 0.44 |
| 1:GD:277:GLY:O | 1:GD:279:ASP:N | 2.50 | 0.44 |
| 1:GE:197:VAL:HG11 | 1:GE:236:PHE:CZ | 2.52 | 0.44 |
| 2:GF:400:ASP:O | 2:GF:424:ARG:NH1 | 2.50 | 0.44 |
| 2:GF:479:TRP:H | 2:GF:479:TRP:HE3 | 1.64 | 0.44 |
| 2:GF:543:LYS:HG2 | 2:GF:575:PHE:CE1 | 2.52 | 0.44 |
| 2:GF:646:ARG:CD | 2:GF:673:GLN:HE22 | 2.13 | 0.44 |
| 2:GF:982:LEU:HD12 | 2:GF:982:LEU:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:134:LEU:HA | 3:GH:134:LEU:HD23 | 1.72 | 0.44 |
| 5:HB:22:GLY:O | 5:HB:26:ILE:N | 2.37 | 0.44 |
| 5:HB:290:SER:CA | 5:HB:371:PHE:H | 2.30 | 0.44 |
| 5:HB:421:ASN:HB2 | 5:HB:434:GLU:CG | 2.47 | 0.44 |
| 5:HC:326:MET:HB2 | 5:HC:326:MET:HE3 | 1.66 | 0.44 |
| 5:HC:34:TYR:OH | 5:HC:42:VAL:N | 2.51 | 0.44 |
| 5:HC:80:ASN:C | 5:HC:81:LEU:HD12 | 2.38 | 0.44 |
| 6:HG:195:LEU:HD13 | 6:HG:215:PHE:CE1 | 2.52 | 0.44 |
| 7:HH:447:HIS:CD2 | 7:HJ:447:HIS:CD2 | 3.05 | 0.44 |
| 7:HI:173:ILE:HD12 | 7:HI:176:ILE:HG21 | 1.98 | 0.44 |
| 7:HI:476:ASP:OD1 | 7:HI:479:ASN:ND2 | 2.40 | 0.44 |
| 7:HH:346:ILE:HD11 | 7:HJ:350:ALA:HB2 | 1.99 | 0.44 |
| 7:HJ:413:ASN:O | 7:HJ:424:ARG:HD3 | 2.17 | 0.44 |
| 5:I:118:LYS:HZ3 | 5:I:147:LYS:HD3 | 1.82 | 0.44 |
| 5:I:290:SER:HA | 5:I:371:PHE:H | 1.82 | 0.44 |
| 8:DE:2:PHE:CD2 | 8:IB:98:GLU:HA | 2.52 | 0.44 |
| 10:ID:221:ALA:O | 10:ID:224:ASN:HB3 | 2.17 | 0.44 |
| 10:ID:286:VAL:HG22 | 10:ID:287:VAL:N | 2.32 | 0.44 |
| 12:IF:122:GLY:O | 12:IF:125:ILE:HG22 | 2.17 | 0.44 |
| 5:J:30:PHE:HE1 | 5:K:30:PHE:HE1 | 1.65 | 0.44 |
| 5:J:80:ASN:C | 5:J:81:LEU:HD12 | 2.38 | 0.44 |
| 5:K:132:ASP:OD2 | 5:K:151:ILE:HA | 2.16 | 0.44 |
| 5:K:322:GLY:O | 5:K:323:THR:OG1 | 2.34 | 0.44 |
| 5:K:293:PHE:HZ | 5:K:366:PRO:O | 2.01 | 0.44 |
| 5:K:469:PRO:HA | 5:K:472:TYR:CZ | 2.52 | 0.44 |
| 5:I:418:GLY:C | 5:K:472:TYR:HB3 | 2.38 | 0.44 |
| 6:M:172:SER:HA | 6:M:176:ILE:O | 2.17 | 0.44 |
| 6:N:107:VAL:HG22 | 6:N:174:TYR:HD2 | 1.82 | 0.44 |
| 6:M:10:VAL:HA | 6:N:13:ARG:HB2 | 1.98 | 0.44 |
| 7:O:132:ARG:O | 7:O:141:VAL:HG12 | 2.17 | 0.44 |
| 7:O:382:ARG:HG3 | 7:O:383:TYR:CD2 | 2.52 | 0.44 |
| 7:O:65:GLU:O | 7:O:69:GLY:N | 2.48 | 0.44 |
| 7:P:171:LYS:HG3 | 6:HE:213:TYR:OH | 2.17 | 0.44 |
| 7:P:228:ILE:O | 7:Q:226:GLY:N | 2.49 | 0.44 |
| 7:P:248:ALA:O | 7:P:252:GLY:N | 2.47 | 0.44 |
| 7:O:265:LEU:N | 7:P:256:THR:O | 2.42 | 0.44 |
| 7:P:32:VAL:HG22 | 7:P:36:ILE:HG12 | 1.99 | 0.44 |
| 7:P:451:PHE:HZ | 7:P:471:THR:HG22 | 1.82 | 0.44 |
| 7:P:77:THR:HA | 7:Q:74:LYS:O | 2.17 | 0.44 |
| 10:U:286:VAL:HG22 | 10:U:287:VAL:N | 2.32 | 0.44 |
| 1:X:172:ILE:HD13 | 1:X:273:ILE:HG12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:345:TYR:OH | 1:X:400:ASN:ND2 | 2.51 | 0.44 |
| 1:X:427:ASN:OD1 | 1:X:428:LYS:N | 2.49 | 0.44 |
| 1:Y:349:VAL:HG13 | 1:Y:392:ILE:HD11 | 1.98 | 0.44 |
| 1:Y:583:SER:OG | 1:Y:584:ASP:N | 2.49 | 0.44 |
| 13:YA:109[D]:ASN:OD1 | 13:YA:110[D]:ARG:N | 2.51 | 0.44 |
| 13:YA:261[A]:LYS:HE2 | 13:YA:293[A]:ASN:HB3 | 1.99 | 0.44 |
| 13:YA:257[C]:LYS:HE2 | 13:YA:266[C]:TRP:CH2 | 2.52 | 0.44 |
| 13:YA:314[F]:SER:OG | 13:YA:316[F]:TRP:HB3 | 2.17 | 0.44 |
| 13:YA:416[B]:HIS:CG | 13:YA:417[B]:PRO:HD2 | 2.51 | 0.44 |
| 13:YA:554[F]:MET:HA | 13:YB:546[F]:VAL:O | 2.16 | 0.44 |
| 13:YA:76[C]:PRO:HB2 | 13:YA:98[C]:GLY:N | 2.32 | 0.44 |
| 13:YB:257[F]:LYS:HE2 | 13:YB:266[F]:TRP:CH2 | 2.52 | 0.44 |
| 13:YB:261[B]:LYS:HE2 | 13:YB:293[B]:ASN:HB3 | 1.99 | 0.44 |
| 13:YB:315[D]:LEU:O | 13:YB:319[D]:GLN:HG2 | 2.16 | 0.44 |
| 13:YB:537[D]:LYS:C | 13:YB:537[D]:LYS:HD3 | 2.37 | 0.44 |
| 13:YB:61[E]:ILE:O | 13:YC:75[E]:GLY:O | 2.35 | 0.44 |
| 13:YC:110[A]:ARG:HD2 | 13:YC:118[A]:THR:O | 2.17 | 0.44 |
| 13:YC:314[C]:SER:OG | 13:YC:316[C]:TRP:HB3 | 2.18 | 0.44 |
| 13:YB:74[E]:THR:HG21 | 13:YC:388[E]:PRO:HB2 | 1.99 | 0.44 |
| 13:YC:537[E]:LYS:HD3 | 13:YC:537[E]:LYS:C | 2.37 | 0.44 |
| 13:YB:551[E]:THR:O | 13:YC:543[E]:ASP:HA | 2.16 | 0.44 |
| 13:YA:122[C]:PRO:HB3 | 13:YC:66[C]:MET:HE2 | 1.98 | 0.44 |
| 13:YC:76[C]:PRO:HB2 | 13:YC:98[C]:GLY:N | 2.32 | 0.44 |
| 14:YD:236[D]:TRP:CD1 | 14:YD:308[D]:ALA:HB2 | 2.51 | 0.44 |
| 14:YD:73[A]:SER:HB2 | 14:YD:85[A]:THR:HG23 | 1.99 | 0.44 |
| 14:YD:88[B]:TYR:HD1 | 14:YD:110[B]:GLY:C | 2.21 | 0.44 |
| 10:U:287:VAL:O | 14:YE:100[A]:LYS:HD3 | 2.17 | 0.44 |
| 14:YE:135[B]:MET:SD | 14:YE:166[B]:PHE:HD1 | 2.40 | 0.44 |
| 14:YE:288[E]:TYR:CE1 | 14:YE:371[E]:LYS:HD3 | 2.52 | 0.44 |
| 14:YE:73[D]:SER:HB2 | 14:YE:85[D]:THR:HG23 | 1.99 | 0.44 |
| 10:GA:287:VAL:O | 14:YF:100[C]:LYS:HD3 | 2.17 | 0.44 |
| 14:YF:135[F]:MET:SD | 14:YF:166[F]:PHE:HD1 | 2.40 | 0.44 |
| 14:YF:73[C]:SER:HB2 | 14:YF:85[C]:THR:HG23 | 1.99 | 0.44 |
| 14:YF:73[D]:SER:HB2 | 14:YF:85[D]:THR:HG23 | 1.99 | 0.44 |
| 14:YF:88[D]:TYR:HD1 | 14:YF:110[D]:GLY:C | 2.21 | 0.44 |
| 2:Z:511:GLU:N | 2:Z:512:PRO:HD2 | 2.33 | 0.44 |
| 2:Z:527:ASN:OD1 | 2:Z:528:ASN:N | 2.50 | 0.44 |
| 2:Z:711:ARG:HD3 | 2:Z:878:ASP:OD1 | 2.18 | 0.44 |
| 1:A:113:THR:HA | 1:A:162:PHE:HB3 | 1.99 | 0.44 |
| 1:A:345:TYR:OH | 1:A:400:ASN:ND2 | 2.51 | 0.44 |
| 1:A:565:GLU:HB3 | 1:A:570:GLN:OE1 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:595:ILE:HG21 | 1:A:602:ILE:HG23 | 1.99 | 0.44 |
| 1:A:642:PHE:HE1 | 1:A:651:LEU:HD13 | 1.81 | 0.44 |
| 4:AB:8:LYS:HD2 | 4:AB:30:LYS:HA | 1.98 | 0.44 |
| 5:AC:104:VAL:HG13 | 5:AC:105:ASN:H | 1.83 | 0.44 |
| 5:AC:312:ARG:HG2 | 5:AC:317:LEU:CA | 2.44 | 0.44 |
| 5:AC:571:GLU:OE2 | 5:AE:567:THR:HG21 | 2.18 | 0.44 |
| 5:AC:90:ASN:HD21 | 5:AD:49:TRP:C | 2.18 | 0.44 |
| 5:AD:361:ASP:H | 5:AD:366:PRO:HB3 | 1.82 | 0.44 |
| 5:AE:115:ASP:OD2 | 5:AE:137:TYR:HE1 | 2.00 | 0.44 |
| 5:AE:290:SER:HB3 | 5:AE:371:PHE:N | 2.33 | 0.44 |
| 5:AE:320:LEU:HG | 5:AE:357:SER:HB3 | 2.00 | 0.44 |
| 6:AF:11:ILE:O | 6:AH:7:LYS:HD2 | 2.17 | 0.44 |
| 7:AI:349:TRP:NE1 | 7:AI:353:SER:O | 2.50 | 0.44 |
| 7:AJ:99:ARG:HG2 | 7:AJ:100:TYR:O | 2.17 | 0.44 |
| 7:AJ:117:THR:HG22 | 7:AJ:120:LYS:NZ | 2.32 | 0.44 |
| 7:AJ:162:PRO:O | 7:AJ:165:THR:N | 2.50 | 0.44 |
| 7:BA:12:GLU:HG3 | 7:BA:15:TYR:H | 1.82 | 0.44 |
| 10:BE:203:ARG:NH1 | 10:BE:311:PHE:HE1 | 2.16 | 0.44 |
| 12:BG:24:CYS:CB | 12:BG:125:ILE:HD13 | 2.46 | 0.44 |
| 1:BH:595:ILE:CG2 | 1:BH:602:ILE:HG23 | 2.47 | 0.44 |
| 1:BH:81:ARG:HA | 1:BH:326:ARG:HG3 | 1.99 | 0.44 |
| 1:BI:121:ASN:HA | 1:BI:155:ARG:HD3 | 1.99 | 0.44 |
| 1:BI:41:ASN:O | 1:BI:42:GLU:HG2 | 2.18 | 0.44 |
| 1:BI:559:ALA:HB3 | 1:BI:562:ASP:OD2 | 2.18 | 0.44 |
| 2:BJ:802:TYR:CE1 | 2:BJ:807:LEU:HB3 | 2.51 | 0.44 |
| 2:BJ:883:VAL:HG13 | 2:BJ:884:HIS:H | 1.82 | 0.44 |
| 2:BJ:865:LYS:HE3 | 2:BJ:893:ILE:HD12 | 1.99 | 0.44 |
| 2:C:515:ASN:OD1 | 2:C:524:CYS:HB3 | 2.17 | 0.44 |
| 2:C:558:HIS:HB2 | 2:C:569:VAL:HG12 | 1.99 | 0.44 |
| 2:C:724:ALA:O | 2:C:725:ARG:HG2 | 2.17 | 0.44 |
| 2:BJ:915:LYS:HG2 | 3:CA:326:GLU:OE2 | 2.17 | 0.44 |
| 3:CA:68:VAL:O | 3:CA:71:MET:HB3 | 2.17 | 0.44 |
| 3:CB:232:GLN:O | 3:CB:233:GLN:HB2 | 2.18 | 0.44 |
| 4:CD:205:THR:OG1 | 4:CE:199:MET:SD | 2.75 | 0.44 |
| 4:CE:107:VAL:O | 4:CE:148:LEU:N | 2.39 | 0.44 |
| 2:BJ:1005:ARG:NH1 | 5:CF:12:ASP:OD2 | 2.50 | 0.44 |
| 5:CF:85:THR:HB | 5:CF:137:TYR:CE2 | 2.52 | 0.44 |
| 5:CF:192:ARG:HG3 | 5:CF:245:GLU:HB2 | 1.99 | 0.44 |
| 5:CF:554:GLY:O | 5:CF:555:CYS:SG | 2.75 | 0.44 |
| 5:CG:361:ASP:H | 5:CG:366:PRO:HB3 | 1.81 | 0.44 |
| 5:CH:103:ASN:CG | 5:CH:104:VAL:H | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:163:ALA:O | 5:CH:246:THR:HG22 | 2.16 | 0.44 |
| 5:CG:7:ILE:HD11 | 5:CH:24:ILE:HD11 | 1.99 | 0.44 |
| 6:CI:172:SER:HA | 6:CI:176:ILE:O | 2.17 | 0.44 |
| 6:CJ:91:SER:OG | 6:CJ:177:THR:HB | 2.18 | 0.44 |
| 3:D:17:ARG:NH1 | 3:D:334:PHE:O | 2.51 | 0.44 |
| 6:DA:73:ASN:ND2 | 6:DA:215:PHE:HE2 | 2.16 | 0.44 |
| 7:DB:97:LEU:HD23 | 7:DD:97:LEU:CD2 | 2.47 | 0.44 |
| 7:DC:99:ARG:HG2 | 7:DC:100:TYR:O | 2.17 | 0.44 |
| 7:DC:111:ASN:ND2 | 7:DC:114:SER:HB3 | 2.32 | 0.44 |
| 7:DC:162:PRO:O | 7:DC:165:THR:N | 2.49 | 0.44 |
| 7:DC:302:ILE:HD12 | 7:DD:306:PHE:CZ | 2.52 | 0.44 |
| 7:DC:445:HIS:CE1 | 7:DD:447:HIS:CE1 | 3.05 | 0.44 |
| 10:DH:37:GLN:HB3 | 10:DH:128:LEU:HB3 | 1.99 | 0.44 |
| 11:DI:73:LEU:HD22 | 11:DI:86:TRP:CH2 | 2.52 | 0.44 |
| 3:E:17:ARG:HD2 | 3:E:334:PHE:OXT | 2.17 | 0.44 |
| 3:D:60:TYR:N | 3:E:9:ARG:HH11 | 2.16 | 0.44 |
| 1:EB:60:LEU:HD23 | 1:EB:60:LEU:HA | 1.73 | 0.44 |
| 2:EC:543:LYS:HG2 | 2:EC:575:PHE:CE1 | 2.52 | 0.44 |
| 2:EC:724:ALA:C | 2:EC:726:PHE:H | 2.20 | 0.44 |
| 3:ED:87:ASP:OD2 | 3:ED:202:ARG:HD2 | 2.17 | 0.44 |
| 2:BJ:483:LYS:HE2 | 3:EE:241:ARG:HH12 | 1.82 | 0.44 |
| 4:EG:145:LYS:N | 4:EG:165:GLU:O | 2.49 | 0.44 |
| 4:EH:22:ASP:O | 4:EH:26:ASP:N | 2.26 | 0.44 |
| 4:EH:67:TYR:CE1 | 4:EH:84:ARG:HD3 | 2.52 | 0.44 |
| 5:EI:290:SER:CA | 5:EI:371:PHE:H | 2.30 | 0.44 |
| 5:EJ:104:VAL:HG22 | 5:EJ:105:ASN:H | 1.83 | 0.44 |
| 5:FA:115:ASP:OD2 | 5:FA:137:TYR:HE1 | 2.00 | 0.44 |
| 5:FA:135:LEU:HA | 5:FA:144:GLU:O | 2.18 | 0.44 |
| 5:FA:323:THR:CG2 | 5:FA:359:GLU:HB2 | 2.47 | 0.44 |
| 5:EJ:551:ILE:HD13 | 5:FA:565:ILE:CD1 | 2.46 | 0.44 |
| 6:FB:107:VAL:HG22 | 6:FB:174:TYR:HD2 | 1.82 | 0.44 |
| 6:FC:91:SER:OG | 6:FC:177:THR:HB | 2.18 | 0.44 |
| 7:FE:132:ARG:O | 7:FE:141:VAL:HG12 | 2.17 | 0.44 |
| 5:AE:351:GLN:HG2 | 7:FE:467:ASN:ND2 | 2.31 | 0.44 |
| 7:FE:17:LYS:H | 7:FG:11:ASN:HB2 | 1.82 | 0.44 |
| 7:FG:413:ASN:O | 7:FG:424:ARG:HD3 | 2.17 | 0.44 |
| 7:FE:447:HIS:CD2 | 7:FG:447:HIS:CD2 | 3.05 | 0.44 |
| 7:FG:359:TRP:CZ2 | 7:FG:524:LYS:HD3 | 2.52 | 0.44 |
| 4:G:146:VAL:HG11 | 4:H:151:ILE:O | 18.71 | 0.44 |
| 4:G:1:MET:HG2 | 4:G:70:HIS:ND1 | 2.32 | 0.44 |
| 1:GD:413:TYR:CE1 | 1:GD:415:PHE:HE1 | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:544:ASP:HB2 | 1:GD:576:ASP:OD2 | 2.16 | 0.44 |
| 1:GE:49:GLU:HA | 1:GE:54:ASN:ND2 | 2.28 | 0.44 |
| 1:GE:634:THR:HB | 1:GE:638:SER:O | 2.17 | 0.44 |
| 1:GE:90:VAL:O | 1:GE:94:GLN:HG2 | 2.17 | 0.44 |
| 2:GF:515:ASN:OD1 | 2:GF:524:CYS:HB3 | 2.17 | 0.44 |
| 1:GD:79:PHE:CE1 | 2:GF:702:GLU:HG2 | 2.52 | 0.44 |
| 2:GF:975:ASN:OD1 | 2:GF:981:GLN:HB3 | 2.17 | 0.44 |
| 3:GG:87:ASP:OD2 | 3:GG:202:ARG:HD2 | 2.17 | 0.44 |
| 3:GH:106:PHE:CD2 | 3:GH:188:TRP:HH2 | 2.35 | 0.44 |
| 3:GG:289:ASN:ND2 | 3:GH:233:GLN:HB2 | 2.31 | 0.44 |
| 3:GG:201:ASN:OD1 | 5:HB:10:VAL:HG21 | 2.17 | 0.44 |
| 5:HB:118:LYS:HZ3 | 5:HB:147:LYS:HD3 | 1.82 | 0.44 |
| 5:HB:468:ASN:O | 5:HB:471:THR:OG1 | 2.27 | 0.44 |
| 5:HC:361:ASP:H | 5:HC:366:PRO:HB3 | 1.81 | 0.44 |
| 5:HD:290:SER:HB3 | 5:HD:371:PHE:N | 2.33 | 0.44 |
| 5:HD:377:HIS:CG | 5:HD:378:GLY:N | 2.85 | 0.44 |
| 6:HE:144:ASN:HB3 | 6:HE:159:THR:HG22 | 1.99 | 0.44 |
| 6:HE:73:ASN:ND2 | 6:HE:215:PHE:HE2 | 2.16 | 0.44 |
| 6:HF:201:VAL:N | 6:HF:210:THR:O | 2.31 | 0.44 |
| 7:HH:12:GLU:HG3 | 7:HH:14:ARG:N | 2.31 | 0.44 |
| 7:HH:349:TRP:NE1 | 7:HH:353:SER:O | 2.50 | 0.44 |
| 7:HH:415:ASN:O | 7:HH:424:ARG:HD2 | 2.17 | 0.44 |
| 7:HH:519:LEU:HA | 7:HI:434:VAL:HG13 | 1.99 | 0.44 |
| 7:HI:451:PHE:HZ | 7:HI:471:THR:HG22 | 1.82 | 0.44 |
| 7:HH:492:PRO:HD2 | 7:HJ:464:ARG:NH2 | 2.32 | 0.44 |
| 8:IA:135:THR:HG22 | 8:IA:156:THR:O | 2.16 | 0.44 |
| 11:IE:5:PHE:CE2 | 11:IE:188:MET:HG2 | 2.52 | 0.44 |
| 11:IE:36:PHE:HZ | 11:IE:76:CYS:SG | 2.40 | 0.44 |
| 5:J:491:ASN:ND2 | 5:J:496:ASP:HB2 | 2.27 | 0.44 |
| 5:K:290:SER:HB3 | 5:K:371:PHE:N | 2.33 | 0.44 |
| 5:K:377:HIS:CG | 5:K:378:GLY:N | 2.85 | 0.44 |
| 6:L:172:SER:HA | 6:L:176:ILE:O | 2.17 | 0.44 |
| 6:L:73:ASN:ND2 | 6:L:215:PHE:HE2 | 2.15 | 0.44 |
| 6:M:195:LEU:HD13 | 6:M:215:PHE:CE1 | 2.52 | 0.44 |
| 7:P:111:ASN:ND2 | 7:P:114:SER:HB3 | 2.32 | 0.44 |
| 7:P:232:THR:HG22 | 7:P:235:GLU:HG3 | 2.00 | 0.44 |
| 7:Q:100:TYR:CE1 | 7:Q:115:SER:HB2 | 2.52 | 0.44 |
| 7:Q:101:SER:OG | 7:Q:105:GLU:HB2 | 2.17 | 0.44 |
| 7:O:463:THR:HG23 | 7:Q:483:PHE:HE1 | 1.82 | 0.44 |
| 10:U:203:ARG:NH1 | 10:U:311:PHE:HE1 | 2.16 | 0.44 |
| 12:W:122:GLY:O | 12:W:125:ILE:HG22 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:113:THR:HA | 1:X:162:PHE:HB3 | 1.99 | 0.44 |
| 1:X:595:ILE:CG2 | 1:X:602:ILE:HG23 | 2.47 | 0.44 |
| 1:Y:182:LEU:O | 1:Y:182:LEU:HD12 | 2.16 | 0.44 |
| 1:Y:40:GLN:HE21 | 1:Y:43:PHE:HB2 | 1.81 | 0.44 |
| 1:Y:470:ASP:O | 1:Y:472:ASP:N | 2.50 | 0.44 |
| 13:YA:109[A]:ASN:OD1 | 13:YA:110[A]:ARG:N | 2.51 | 0.44 |
| 13:YA:236[D]:ILE:HG23 | 13:YA:240[D]:GLU:HB2 | 2.00 | 0.44 |
| 13:YA:252[A]:MET:HB3 | 13:YA:252[A]:MET:HE3 | 1.83 | 0.44 |
| 13:YA:394[A]:GLU:N | 13:YC:70[A]:GLY:O | 2.50 | 0.44 |
| 13:YA:450[B]:VAL:O | 13:YC:459[B]:GLY:N | 2.51 | 0.44 |
| 13:YA:537[C]:LYS:C | 13:YA:537[C]:LYS:HD3 | 2.37 | 0.44 |
| 13:YB:146[B]:VAL:O | 13:YB:150[B]:SER:OG | 2.34 | 0.44 |
| 13:YB:537[F]:LYS:C | 13:YB:537[F]:LYS:HD3 | 2.37 | 0.44 |
| 13:YA:554[A]:MET:HA | 13:YB:546[A]:VAL:O | 2.16 | 0.44 |
| 13:YB:552[B]:GLU:HB2 | 13:YC:544[B]:TRP:HB2 | 1.98 | 0.44 |
| 13:YA:61[B]:ILE:HD11 | 13:YB:72[B]:SER:O | 2.17 | 0.44 |
| 13:YC:110[B]:ARG:HD2 | 13:YC:118[B]:THR:O | 2.17 | 0.44 |
| 13:YC:110[E]:ARG:HD2 | 13:YC:118[E]:THR:O | 2.17 | 0.44 |
| 13:YB:67[C]:SER:HB3 | 13:YC:123[C]:ARG:HB2 | 1.99 | 0.44 |
| 13:YC:261[C]:LYS:HE2 | 13:YC:293[C]:ASN:HB3 | 1.99 | 0.44 |
| 13:YC:36[F]:PRO:HB2 | 13:YC:38[F]:GLN:OE1 | 2.17 | 0.44 |
| 13:YC:490[B]:VAL:HG12 | 13:YC:492[B]:GLY:H | 1.81 | 0.44 |
| 13:YC:521[D]:LEU:HD12 | 13:YC:522[D]:VAL:N | 2.32 | 0.44 |
| 13:YC:537[B]:LYS:HD3 | 13:YC:537[B]:LYS:C | 2.37 | 0.44 |
| 13:YA:534[E]:LEU:CB | 13:YC:538[E]:VAL:HG11 | 2.47 | 0.44 |
| 13:YB:567[D]:ILE:HG23 | 13:YC:565[D]:TYR:CD2 | 2.50 | 0.44 |
| 10:U:287:VAL:O | 14:YD:100[C]:LYS:HD3 | 2.18 | 0.44 |
| 13:YA:47[A]:ILE:HG12 | 14:YD:123[A]:PRO:HD3 | 1.98 | 0.44 |
| 14:YD:277[A]:VAL:HG11 | 14:YD:294[A]:GLU:HG2 | 1.99 | 0.44 |
| 14:YD:279[E]:ARG:HA | 14:YD:279[E]:ARG:HD3 | 1.43 | 0.44 |
| 14:YD:277[B]:VAL:HG11 | 14:YD:294[B]:GLU:HG2 | 1.99 | 0.44 |
| 14:YD:73[F]:SER:HA | 14:YD:85[F]:THR:HA | 1.99 | 0.44 |
| 14:YD:73[F]:SER:HB2 | 14:YD:85[F]:THR:HG23 | 1.99 | 0.44 |
| 14:YE:135[D]:MET:SD | 14:YE:166[D]:PHE:HD1 | 2.40 | 0.44 |
| 14:YE:279[D]:ARG:HA | 14:YE:279[D]:ARG:HD3 | 1.43 | 0.44 |
| 14:YE:288[F]:TYR:CE1 | 14:YE:371[F]:LYS:HD3 | 2.52 | 0.44 |
| 14:YE:360[A]:ASN:N | 14:YE:360[A]:ASN:HD22 | 1.98 | 0.44 |
| 14:YE:364[C]:LEU:HA | 14:YE:364[C]:LEU:HD22 | 1.79 | 0.44 |
| 14:YE:288[B]:TYR:CE1 | 14:YE:371[B]:LYS:HD3 | 2.52 | 0.44 |
| 13:YC:47[C]:ILE:HG12 | 14:YF:123[C]:PRO:HD3 | 1.98 | 0.44 |
| 14:YF:140[E]:TYR:HE2 | 14:YF:148[E]:PRO:HD3 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:15[E]:LYS:HB3 | 14:YF:15[E]:LYS:HE2 | 1.54 | 0.44 |
| 14:YF:135[B]:MET:SD | 14:YF:166[B]:PHE:HD1 | 2.40 | 0.44 |
| 14:YD:91[F]:LYS:O | 14:YF:242[F]:PRO:HD2 | 2.17 | 0.44 |
| 14:YF:266[D]:ILE:HD11 | 14:YF:290[D]:ASN:CG | 2.37 | 0.44 |
| 14:YF:364[A]:LEU:HD22 | 14:YF:364[A]:LEU:HA | 1.79 | 0.44 |
| 14:YF:88[C]:TYR:HD1 | 14:YF:110[C]:GLY:C | 2.21 | 0.44 |
| 2:Z:612:TRP:CD1 | 2:Z:618:PHE:HB3 | 2.53 | 0.44 |
| 2:Z:724:ALA:O | 2:Z:725:ARG:HG2 | 2.17 | 0.44 |
| 2:Z:737:THR:HB | 2:Z:740:ILE:HD12 | 1.98 | 0.44 |
| 2:Z:878:ASP:O | 2:Z:881:ARG:N | 2.49 | 0.44 |
| 2:Z:952:ILE:HG13 | 2:Z:952:ILE:H | 1.47 | 0.44 |
| 1:A:7:ASN:OD1 | 1:A:7:ASN:N | 2.50 | 0.44 |
| 5:AC:262:GLN:HA | 5:AC:381:ILE:O | 2.17 | 0.44 |
| 5:AC:421:ASN:HB2 | 5:AC:434:GLU:CG | 2.47 | 0.44 |
| 5:AC:518:GLY:N | 5:AE:594:THR:OG1 | 2.50 | 0.44 |
| 5:AD:304:ILE:HD11 | 5:AD:309:LEU:HA | 2.00 | 0.44 |
| 5:AD:302:GLU:HB3 | 5:AD:365:ILE:CD1 | 2.47 | 0.44 |
| 5:AE:137:TYR:HA | 5:AE:143:TRP:HD1 | 1.81 | 0.44 |
| 5:AE:163:ALA:O | 5:AE:246:THR:HG22 | 2.16 | 0.44 |
| 5:AE:293:PHE:HZ | 5:AE:366:PRO:O | 2.00 | 0.44 |
| 6:AF:195:LEU:HD13 | 6:AF:215:PHE:CE1 | 2.52 | 0.44 |
| 6:AG:144:ASN:HB3 | 6:AG:159:THR:HG22 | 1.99 | 0.44 |
| 6:AH:108:LEU:HD23 | 6:AH:113:PRO:HA | 2.00 | 0.44 |
| 7:AI:63:GLU:O | 7:AI:67:ILE:HG12 | 2.18 | 0.44 |
| 1:A:69:GLN:CD | 1:B:21:PHE:HZ | 2.20 | 0.44 |
| 1:B:491:PHE:HE2 | 1:B:619:GLN:HA | 1.82 | 0.44 |
| 7:BA:493:GLU:HA | 7:BA:496:ARG:NH2 | 2.32 | 0.44 |
| 9:BD:114:ASP:O | 11:DI:47:THR:OG1 | 2.34 | 0.44 |
| 12:BG:22:PHE:CG | 12:DJ:228:LEU:HD13 | 2.52 | 0.44 |
| 1:BH:446:ARG:NE | 1:BH:450:GLU:OE2 | 2.51 | 0.44 |
| 1:BH:554:ILE:HG22 | 1:BH:555:ILE:O | 2.16 | 0.44 |
| 1:BH:619:GLN:H | 1:BH:619:GLN:CD | 2.18 | 0.44 |
| 1:BI:358:GLN:HB2 | 1:BI:379:LYS:HD3 | 2.00 | 0.44 |
| 2:BJ:467:LEU:HD11 | 3:ED:56:PHE:N | 2.32 | 0.44 |
| 2:BJ:515:ASN:OD1 | 2:BJ:524:CYS:HB3 | 2.17 | 0.44 |
| 2:BJ:558:HIS:HB2 | 2:BJ:569:VAL:HG12 | 1.99 | 0.44 |
| 2:BJ:934:ALA:H | 2:BJ:997:SER:CB | 2.31 | 0.44 |
| 2:C:202:PHE:HB3 | 2:C:209:VAL:HG22 | 1.98 | 0.44 |
| 2:C:209:VAL:O | 2:C:221:ALA:HA | 2.16 | 0.44 |
| 2:C:336:ILE:HG21 | 2:C:350:PHE:O | 2.17 | 0.44 |
| 2:C:479:TRP:CD1 | 2:C:505:PRO:O | 2.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:543:LYS:HG2 | 2:C:575:PHE:CE1 | 2.52 | 0.44 |
| 2:BJ:1020:ARG:NH2 | 3:CA:94:ASP:OD2 | 2.51 | 0.44 |
| 4:CC:107:VAL:O | 4:CC:148:LEU:N | 2.39 | 0.44 |
| 4:CC:152:SER:O | 4:CC:158:SER:HA | 2.18 | 0.44 |
| 4:CC:68:GLN:HB3 | 4:CC:70:HIS:NE2 | 2.32 | 0.44 |
| 4:CC:67:TYR:CE1 | 4:CC:84:ARG:HD3 | 2.52 | 0.44 |
| 4:CD:152:SER:O | 4:CD:158:SER:HA | 2.18 | 0.44 |
| 4:CD:68:GLN:HB3 | 4:CD:70:HIS:NE2 | 2.32 | 0.44 |
| 4:CD:67:TYR:CE1 | 4:CD:84:ARG:HD3 | 2.52 | 0.44 |
| 5:CF:104:VAL:HG13 | 5:CF:105:ASN:H | 1.83 | 0.44 |
| 5:CF:248:MET:HB2 | 5:CF:254:TRP:CD1 | 2.52 | 0.44 |
| 5:CF:421:ASN:HB2 | 5:CF:434:GLU:CG | 2.47 | 0.44 |
| 5:CG:80:ASN:C | 5:CG:81:LEU:HD12 | 2.38 | 0.44 |
| 5:CG:71:ASN:HB2 | 5:CG:99:PHE:HZ | 1.82 | 0.44 |
| 5:CH:202:TYR:CE1 | 5:CH:206:PHE:HD1 | 2.35 | 0.44 |
| 6:CI:91:SER:OG | 6:CI:177:THR:HB | 2.18 | 0.44 |
| 6:CI:198:ALA:O | 6:CJ:203:LEU:HB3 | 2.17 | 0.44 |
| 7:DB:479:ASN:O | 7:DC:468:PHE:HB2 | 2.16 | 0.44 |
| 7:DB:63:GLU:O | 7:DB:67:ILE:HG12 | 2.18 | 0.44 |
| 7:DD:77:THR:HG23 | 7:DD:79:ALA:H | 1.80 | 0.44 |
| 8:DE:118:ARG:HE | 8:DF:62:GLY:HA2 | 1.82 | 0.44 |
| 10:DH:221:ALA:O | 10:DH:224:ASN:HB3 | 2.17 | 0.44 |
| 3:E:40:THR:OG1 | 3:E:273:SER:HB3 | 2.17 | 0.44 |
| 1:EA:172:ILE:HD13 | 1:EA:273:ILE:HG12 | 1.99 | 0.44 |
| 1:EA:288:TYR:CE2 | 1:EA:290:ASP:O | 2.70 | 0.44 |
| 1:EB:332:LYS:O | 1:EB:335:THR:HG22 | 2.18 | 0.44 |
| 2:EC:479:TRP:H | 2:EC:479:TRP:HE3 | 1.64 | 0.44 |
| 2:EC:6:PRO:O | 2:EC:7:SER:OG | 2.27 | 0.44 |
| 3:ED:17:ARG:NH1 | 3:ED:334:PHE:O | 2.51 | 0.44 |
| 3:ED:47:TRP:HH2 | 3:ED:58:PRO:HB3 | 1.82 | 0.44 |
| 3:EE:197:ASP:OD1 | 3:EE:198:VAL:N | 2.48 | 0.44 |
| 4:EF:63:ALA:HB3 | 4:EG:83:THR:HA | 1.99 | 0.44 |
| 4:EH:152:SER:O | 4:EH:158:SER:HA | 2.18 | 0.44 |
| 5:EI:288:MET:HG2 | 5:EI:289:LYS:O | 2.18 | 0.44 |
| 5:EI:293:PHE:HA | 5:EI:295:ALA:H | 1.82 | 0.44 |
| 5:EI:361:ASP:N | 5:EI:365:ILE:O | 2.50 | 0.44 |
| 5:EJ:480:LEU:HD23 | 5:EJ:480:LEU:HA | 1.81 | 0.44 |
| 4:F:152:SER:O | 4:F:158:SER:HA | 2.18 | 0.44 |
| 5:FA:202:TYR:CE1 | 5:FA:206:PHE:HD1 | 2.35 | 0.44 |
| 5:FA:163:ALA:O | 5:FA:246:THR:HG22 | 2.16 | 0.44 |
| 5:EI:571:GLU:OE2 | 5:FA:567:THR:HG21 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FD:144:ASN:HB3 | 6:FD:159:THR:HG22 | 1.99 | 0.44 |
| 7:FE:59:PHE:HB2 | 7:FE:74:LYS:HG2 | 1.99 | 0.44 |
| 7:FF:162:PRO:O | 7:FF:165:THR:N | 2.49 | 0.44 |
| 7:FG:133:VAL:HA | 7:FG:141:VAL:O | 2.18 | 0.44 |
| 8:FI:114:ARG:HD2 | 8:FI:123:VAL:HG11 | 1.97 | 0.44 |
| 8:FI:98:GLU:N | 8:FI:98:GLU:OE1 | 2.48 | 0.44 |
| 11:GB:32:TYR:HA | 11:GB:35:TYR:CD2 | 2.52 | 0.44 |
| 12:GC:220:SER:HA | 12:GC:243:PHE:HD1 | 1.82 | 0.44 |
| 1:GD:200:TYR:HB2 | 1:GD:269:VAL:HG13 | 1.98 | 0.44 |
| 1:GD:288:TYR:CE2 | 1:GD:290:ASP:O | 2.70 | 0.44 |
| 1:GD:336:GLN:HG3 | 1:GD:337:GLN:N | 2.31 | 0.44 |
| 2:GF:711:ARG:HD3 | 2:GF:878:ASP:OD1 | 2.18 | 0.44 |
| 2:GF:883:VAL:HG13 | 2:GF:884:HIS:H | 1.82 | 0.44 |
| 3:GG:17:ARG:NH1 | 3:GG:334:PHE:O | 2.51 | 0.44 |
| 4:GJ:111:ASN:HB2 | 4:GJ:116:ILE:HD12 | 1.99 | 0.44 |
| 5:HB:323:THR:HG21 | 5:HB:354:THR:HG23 | 1.98 | 0.44 |
| 5:HC:104:VAL:HG22 | 5:HC:105:ASN:H | 1.83 | 0.44 |
| 5:HC:135:LEU:HA | 5:HC:144:GLU:O | 2.18 | 0.44 |
| 5:HC:323:THR:HB | 5:HC:355:ASP:HB3 | 1.99 | 0.44 |
| 5:HC:466:PRO:HA | 5:HC:596:TYR:CZ | 2.52 | 0.44 |
| 5:HC:469:PRO:HA | 5:HC:472:TYR:CZ | 2.52 | 0.44 |
| 5:HD:320:LEU:HG | 5:HD:357:SER:HB3 | 2.00 | 0.44 |
| 5:HD:339:GLU:HB3 | 6:HE:172:SER:C | 2.37 | 0.44 |
| 6:HE:107:VAL:HG22 | 6:HE:174:TYR:HD2 | 1.82 | 0.44 |
| 6:HG:91:SER:OG | 6:HG:177:THR:HB | 2.18 | 0.44 |
| 6:FB:77:VAL:CG2 | 7:HI:167:GLN:HE21 | 2.28 | 0.44 |
| 7:HI:165:THR:HA | 7:HI:168:LEU:HB2 | 1.99 | 0.44 |
| 7:HI:417:ASN:HB3 | 7:HI:421:GLY:HA2 | 1.99 | 0.44 |
| 7:HI:100:TYR:OH | 7:HJ:113:GLU:O | 2.05 | 0.44 |
| 7:HH:97:LEU:HD23 | 7:HJ:97:LEU:CD2 | 2.48 | 0.44 |
| 5:I:104:VAL:HG13 | 5:I:105:ASN:H | 1.83 | 0.44 |
| 5:I:267:ASP:CG | 5:I:285:LEU:HB2 | 2.38 | 0.44 |
| 8:IB:22:GLN:OE1 | 8:IB:116:TYR:OH | 2.25 | 0.44 |
| 8:IB:32:PHE:O | 8:IB:35:GLN:N | 2.50 | 0.44 |
| 9:IC:79:SER:OG | 10:ID:121:LYS:O | 2.35 | 0.44 |
| 5:K:192:ARG:HB2 | 5:K:245:GLU:HB2 | 1.99 | 0.44 |
| 6:M:107:VAL:HG22 | 6:M:174:TYR:HD2 | 1.82 | 0.44 |
| 6:N:91:SER:OG | 6:N:177:THR:HB | 2.18 | 0.44 |
| 6:L:73:ASN:HB3 | 6:N:69:THR:HA | 2.00 | 0.44 |
| 6:N:71:ILE:O | 6:N:215:PHE:N | 2.36 | 0.44 |
| 7:O:408:HIS:CE1 | 7:Q:437:VAL:HG21 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:P:126:ASN:O | 7:P:129:PHE:HB3 | 2.18 | 0.44 |
| 7:P:26:PRO:HA | 7:P:27:PRO:HD3 | 1.72 | 0.44 |
| 11:V:32:TYR:HA | 11:V:35:TYR:CD2 | 2.52 | 0.44 |
| 1:X:510:MET:HE3 | 1:X:623:LEU:HD11 | 2.00 | 0.44 |
| 1:Y:121:ASN:HA | 1:Y:155:ARG:HD3 | 1.98 | 0.44 |
| 1:Y:346:ASP:O | 1:Y:350:SER:N | 2.50 | 0.44 |
| 1:Y:358:GLN:HB2 | 1:Y:379:LYS:HD3 | 1.99 | 0.44 |
| 13:YA:110[B]:ARG:HD2 | 13:YA:118[B]:THR:O | 2.17 | 0.44 |
| 13:YA:110[D]:ARG:HD2 | 13:YA:118[D]:THR:O | 2.17 | 0.44 |
| 13:YA:112[B]:GLU:C | 13:YA:115[B]:SER:HB3 | 2.38 | 0.44 |
| 13:YA:36[D]:PRO:HB2 | 13:YA:38[D]:GLN:OE1 | 2.17 | 0.44 |
| 13:YA:376[A]:PHE:CD2 | 13:YB:447[A]:ASN:OD1 | 2.71 | 0.44 |
| 13:YA:36[F]:PRO:HB2 | 13:YA:38[F]:GLN:OE1 | 2.17 | 0.44 |
| 13:YA:450[E]:VAL:O | 13:YC:459[E]:GLY:N | 2.51 | 0.44 |
| 13:YA:516[B]:GLY:O | 13:YC:522[B]:VAL:HG23 | 2.17 | 0.44 |
| 13:YA:537[F]:LYS:HD3 | 13:YA:537[F]:LYS:C | 2.37 | 0.44 |
| 13:YA:543[C]:ASP:HA | 13:YC:551[C]:THR:O | 2.17 | 0.44 |
| 13:YA:558[E]:SER:N | 13:YB:550[E]:TRP:O | 2.50 | 0.44 |
| 13:YA:66[B]:MET:HE2 | 13:YB:122[B]:PRO:HB3 | 1.98 | 0.44 |
| 13:YB:109[C]:ASN:OD1 | 13:YB:111[C]:LEU:N | 2.50 | 0.44 |
| 13:YB:109[F]:ASN:OD1 | 13:YB:111[F]:LEU:N | 2.50 | 0.44 |
| 13:YB:116[F]:ASP:OD2 | 13:YB:121[F]:TYR:N | 2.43 | 0.44 |
| 13:YB:147[F]:ILE:HD11 | 13:YB:188[F]:LEU:HG | 2.00 | 0.44 |
| 13:YB:24[D]:LEU:HD21 | 13:YC:102[D]:GLY:HA2 | 1.99 | 0.44 |
| 13:YB:314[A]:SER:OG | 13:YB:316[A]:TRP:HB3 | 2.17 | 0.44 |
| 13:YB:315[C]:LEU:O | 13:YB:319[C]:GLN:HG2 | 2.16 | 0.44 |
| 13:YB:321[D]:LYS:HD3 | 13:YC:452[D]:GLY:CA | 2.46 | 0.44 |
| 13:YB:36[A]:PRO:HB2 | 13:YB:38[A]:GLN:OE1 | 2.17 | 0.44 |
| 13:YB:521[F]:LEU:HD12 | 13:YB:522[F]:VAL:N | 2.32 | 0.44 |
| 13:YB:537[E]:LYS:C | 13:YB:537[E]:LYS:HD3 | 2.37 | 0.44 |
| 13:YB:7[C]:ASN:HD22 | 13:YB:8[C]:LEU:HG | 1.81 | 0.44 |
| 13:YC:112[B]:GLU:C | 13:YC:115[B]:SER:HB3 | 2.38 | 0.44 |
| 13:YC:147[D]:ILE:HD11 | 13:YC:188[D]:LEU:HG | 2.00 | 0.44 |
| 13:YC:266[A]:TRP:CD1 | 13:YC:274[A]:GLN:HG2 | 2.52 | 0.44 |
| 13:YC:314[E]:SER:OG | 13:YC:316[E]:TRP:HB3 | 2.17 | 0.44 |
| 13:YC:534[B]:LEU:HD11 | 13:YC:536[B]:TRP:NE1 | 2.32 | 0.44 |
| 13:YC:534[E]:LEU:HD11 | 13:YC:536[E]:TRP:NE1 | 2.32 | 0.44 |
| 13:YC:537[C]:LYS:C | 13:YC:537[C]:LYS:HD3 | 2.37 | 0.44 |
| 13:YB:552[C]:GLU:HB2 | 13:YC:544[C]:TRP:HB2 | 1.98 | 0.44 |
| 14:YD:140[C]:TYR:HE2 | 14:YD:148[C]:PRO:HD3 | 1.82 | 0.44 |
| 14:YD:140[E]:TYR:HE2 | 14:YD:148[E]:PRO:HD3 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:140[F]:TYR:HE2 | 14:YD:148[F]:PRO:HD3 | 1.82 | 0.44 |
| 14:YD:135[F]:MET:SD | 14:YD:166[F]:PHE:HD1 | 2.40 | 0.44 |
| 14:YD:233[A]:ASP:N | 14:YD:233[A]:ASP:OD1 | 2.51 | 0.44 |
| 14:YD:233[F]:ASP:OD1 | 14:YD:233[F]:ASP:N | 2.51 | 0.44 |
| 14:YD:277[C]:VAL:HG11 | 14:YD:294[C]:GLU:HG2 | 1.99 | 0.44 |
| 14:YD:88[A]:TYR:HD1 | 14:YD:110[A]:GLY:C | 2.21 | 0.44 |
| 14:YD:91[A]:LYS:O | 14:YF:242[A]:PRO:HD2 | 2.17 | 0.44 |
| 13:YB:26[B]:ARG:HD3 | 14:YE:259[B]:LEU:CD2 | 2.48 | 0.44 |
| 14:YE:266[E]:ILE:HD11 | 14:YE:290[E]:ASN:CG | 2.37 | 0.44 |
| 14:YE:288[C]:TYR:CE1 | 14:YE:371[C]:LYS:HD3 | 2.53 | 0.44 |
| 14:YF:117[E]:ASN:O | 14:YF:119[E]:LYS:HG3 | 2.17 | 0.44 |
| 14:YF:140[C]:TYR:HE2 | 14:YF:148[C]:PRO:HD3 | 1.82 | 0.44 |
| 14:YF:86[D]:ARG:HD2 | 14:YF:192[D]:ILE:HD12 | 2.00 | 0.44 |
| 14:YF:307[F]:TYR:HA | 14:YF:307[F]:TYR:HD1 | 1.66 | 0.44 |
| 14:YF:73[B]:SER:HA | 14:YF:85[B]:THR:HA | 1.99 | 0.44 |
| 14:YF:88[B]:TYR:HD1 | 14:YF:110[B]:GLY:C | 2.21 | 0.44 |
| 2:Z:138:ASN:O | 2:Z:555:ARG:CZ | 2.64 | 0.44 |
| 2:Z:548:ILE:HG21 | 2:Z:555:ARG:N | 2.32 | 0.44 |
| 2:Z:883:VAL:HG13 | 2:Z:884:HIS:H | 1.82 | 0.44 |
| 4:AA:145:LYS:N | 4:AA:165:GLU:O | 2.49 | 0.44 |
| 4:AA:8:LYS:HD2 | 4:AA:30:LYS:HA | 1.98 | 0.44 |
| 4:AB:192:PHE:CE1 | 4:AB:197:TYR:HB2 | 2.53 | 0.44 |
| 5:AC:192:ARG:HG3 | 5:AC:245:GLU:HB2 | 1.99 | 0.44 |
| 5:AC:275:SER:HA | 5:AC:280:ILE:HG22 | 2.00 | 0.44 |
| 5:AD:146:VAL:HG11 | 5:AE:151:ILE:O | 2.17 | 0.44 |
| 5:AD:30:PHE:HE1 | 5:AE:30:PHE:HE1 | 1.65 | 0.44 |
| 5:AC:317:LEU:HD13 | 5:AD:312:ARG:HH12 | 1.83 | 0.44 |
| 5:AD:34:TYR:OH | 5:AD:42:VAL:N | 2.51 | 0.44 |
| 5:AE:176:ASP:HA | 5:AE:231:ARG:HA | 1.99 | 0.44 |
| 6:AF:144:ASN:HB3 | 6:AF:159:THR:HG22 | 1.99 | 0.44 |
| 6:AH:172:SER:HA | 6:AH:176:ILE:O | 2.17 | 0.44 |
| 6:AF:204:ASP:N | 6:AH:198:ALA:O | 2.29 | 0.44 |
| 6:AH:73:ASN:ND2 | 6:AH:215:PHE:HE2 | 2.16 | 0.44 |
| 7:AI:87:TYR:HB3 | 7:AI:88:PRO:HD3 | 1.99 | 0.44 |
| 7:AJ:111:ASN:ND2 | 7:AJ:114:SER:HB3 | 2.32 | 0.44 |
| 7:AI:162:PRO:CB | 7:AJ:150:ALA:HA | 2.47 | 0.44 |
| 7:AI:257:THR:HA | 7:BA:265:LEU:O | 2.18 | 0.44 |
| 7:AI:39:ILE:HD13 | 7:BA:39:ILE:HD13 | 1.99 | 0.44 |
| 7:BA:407:SER:HA | 7:BA:410:THR:OG1 | 2.17 | 0.44 |
| 7:BA:88:PRO:HG2 | 7:BA:95:TYR:O | 2.16 | 0.44 |
| 8:BC:69:TRP:CZ3 | 8:BC:157:LEU:HD12 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:BG:122:GLY:O | 12:BG:125:ILE:HG22 | 2.17 | 0.44 |
| 1:BI:197:VAL:HG11 | 1:BI:236:PHE:CZ | 2.52 | 0.44 |
| 2:BJ:380:ILE:O | 2:BJ:401:LYS:HA | 2.17 | 0.44 |
| 2:BJ:369:ASP:HB2 | 2:BJ:434:MET:HG2 | 1.99 | 0.44 |
| 2:BJ:748:PHE:CD2 | 2:BJ:756:VAL:HG11 | 2.52 | 0.44 |
| 2:BJ:711:ARG:HD3 | 2:BJ:878:ASP:OD1 | 2.17 | 0.44 |
| 2:C:527:ASN:OD1 | 2:C:528:ASN:N | 2.50 | 0.44 |
| 2:C:562:ASP:O | 2:C:565:ASP:N | 2.44 | 0.44 |
| 2:C:613:LYS:O | 2:C:615:THR:N | 2.47 | 0.44 |
| 3:CA:294:LYS:N | 3:CA:297:TYR:OH | 2.42 | 0.44 |
| 4:CE:67:TYR:CE1 | 4:CE:84:ARG:HD3 | 2.52 | 0.44 |
| 5:CF:103:ASN:O | 5:CF:104:VAL:C | 2.55 | 0.44 |
| 5:CG:120:SER:OG | 5:CG:122:VAL:HG22 | 2.16 | 0.44 |
| 5:CG:1:MET:H3 | 5:CH:41:ASP:HB3 | 1.83 | 0.44 |
| 5:CG:58:GLN:N | 5:CG:58:GLN:OE1 | 2.42 | 0.44 |
| 5:CG:49:TRP:CZ3 | 5:CG:96:ARG:HD2 | 2.52 | 0.44 |
| 5:CH:135:LEU:HA | 5:CH:144:GLU:O | 2.18 | 0.44 |
| 5:CG:30:PHE:HE1 | 5:CH:30:PHE:HE1 | 1.65 | 0.44 |
| 6:DA:107:VAL:HG22 | 6:DA:174:TYR:HD2 | 1.82 | 0.44 |
| 7:DB:132:ARG:O | 7:DB:141:VAL:HG12 | 2.17 | 0.44 |
| 7:DB:94:VAL:HG12 | 7:DB:95:TYR:O | 2.18 | 0.44 |
| 7:DC:110:VAL:HG12 | 7:DC:111:ASN:N | 2.33 | 0.44 |
| 7:DD:67:ILE:HA | 7:DD:84:ARG:NH2 | 2.31 | 0.44 |
| 8:BC:61:ALA:HB2 | 8:DF:133:TRP:CH2 | 2.53 | 0.44 |
| 12:DJ:24:CYS:CB | 12:DJ:125:ILE:HD13 | 2.47 | 0.44 |
| 1:EA:113:THR:HA | 1:EA:162:PHE:HB3 | 1.99 | 0.44 |
| 1:EA:81:ARG:HA | 1:EA:326:ARG:HG3 | 1.99 | 0.44 |
| 1:EB:197:VAL:HG11 | 1:EB:236:PHE:CZ | 2.52 | 0.44 |
| 1:EB:451:ASP:O | 1:EB:454:ILE:HD12 | 2.17 | 0.44 |
| 2:EC:549:PRO:HB2 | 2:EC:550:GLU:OE1 | 2.17 | 0.44 |
| 2:EC:612:TRP:CD1 | 2:EC:618:PHE:HB3 | 2.53 | 0.44 |
| 2:EC:921:TRP:N | 2:EC:921:TRP:CD1 | 2.85 | 0.44 |
| 2:EC:975:ASN:OD1 | 2:EC:981:GLN:HB3 | 2.17 | 0.44 |
| 2:BJ:473:TYR:HB2 | 3:ED:59:PRO:HB2 | 1.99 | 0.44 |
| 3:EE:178:GLY:O | 3:EE:180:ILE:N | 2.51 | 0.44 |
| 3:EE:232:GLN:O | 3:EE:233:GLN:HB2 | 2.18 | 0.44 |
| 4:EF:67:TYR:CE1 | 4:EF:84:ARG:HD3 | 2.52 | 0.44 |
| 5:EJ:34:TYR:O | 5:EJ:38:GLY:N | 2.37 | 0.44 |
| 5:FA:103:ASN:CG | 5:FA:104:VAL:H | 2.20 | 0.44 |
| 5:FA:131:SER:HA | 5:FA:150:GLN:HA | 1.99 | 0.44 |
| 5:FA:290:SER:HB3 | 5:FA:371:PHE:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FB:144:ASN:HB3 | 6:FB:159:THR:HG22 | 1.99 | 0.44 |
| 6:FB:172:SER:HA | 6:FB:176:ILE:O | 2.17 | 0.44 |
| 6:FD:91:SER:OG | 6:FD:177:THR:HB | 2.18 | 0.44 |
| 7:FE:63:GLU:O | 7:FE:67:ILE:HG12 | 2.18 | 0.44 |
| 7:FE:94:VAL:HG12 | 7:FE:95:TYR:O | 2.18 | 0.44 |
| 7:FF:335:ASN:H | 7:FG:329:ASN:HD21 | 1.66 | 0.44 |
| 7:FF:347:MET:HE3 | 7:FF:347:MET:HB2 | 1.77 | 0.44 |
| 4:G:152:SER:O | 4:G:158:SER:HA | 2.18 | 0.44 |
| 4:G:67:TYR:CE1 | 4:G:84:ARG:HD3 | 2.52 | 0.44 |
| 12:GC:99:SER:HB3 | 12:GC:102:GLY:O | 2.17 | 0.44 |
| 1:GD:116:ASP:OD1 | 1:GD:118:LEU:N | 2.46 | 0.44 |
| 1:GE:276:ASN:HB2 | 1:GE:279:ASP:OD2 | 2.18 | 0.44 |
| 1:GE:50:GLY:HA2 | 2:GF:657:TYR:OH | 2.17 | 0.44 |
| 1:GE:60:LEU:HD23 | 1:GE:60:LEU:HA | 1.73 | 0.44 |
| 2:GF:110:PHE:HB3 | 2:GF:621:ALA:HA | 1.99 | 0.44 |
| 2:GF:380:ILE:O | 2:GF:401:LYS:HA | 2.17 | 0.44 |
| 2:GF:612:TRP:CD1 | 2:GF:618:PHE:HB3 | 2.53 | 0.44 |
| 2:GF:675:LEU:HA | 2:GF:675:LEU:HD12 | 1.67 | 0.44 |
| 4:GI:192:PHE:CE1 | 4:GI:197:TYR:HB2 | 2.53 | 0.44 |
| 4:H:68:GLN:HB3 | 4:H:70:HIS:NE2 | 2.32 | 0.44 |
| 4:HA:8:LYS:HD2 | 4:HA:30:LYS:HA | 1.97 | 0.44 |
| 5:HB:573:LYS:HD3 | 5:HC:537:THR:O | 2.16 | 0.44 |
| 5:HD:103:ASN:CG | 5:HD:104:VAL:H | 2.20 | 0.44 |
| 5:HD:135:LEU:HA | 5:HD:144:GLU:O | 2.18 | 0.44 |
| 5:HB:312:ARG:CZ | 5:HD:317:LEU:HD13 | 2.48 | 0.44 |
| 5:HD:470:VAL:O | 5:HD:474:GLY:N | 2.50 | 0.44 |
| 5:HB:555:CYS:O | 5:HD:557:TYR:HE1 | 2.01 | 0.44 |
| 7:HH:382:ARG:HG3 | 7:HH:383:TYR:CD2 | 2.52 | 0.44 |
| 7:HH:63:GLU:O | 7:HH:67:ILE:HG12 | 2.18 | 0.44 |
| 7:HH:87:TYR:HB3 | 7:HH:88:PRO:HD3 | 1.99 | 0.44 |
| 7:HI:116:ILE:HG23 | 7:HI:120:LYS:HB2 | 2.00 | 0.44 |
| 7:HI:248:ALA:O | 7:HI:252:GLY:N | 2.47 | 0.44 |
| 7:HI:418:ASP:HA | 7:HI:424:ARG:NH2 | 2.32 | 0.44 |
| 8:IA:32:PHE:O | 8:IA:35:GLN:N | 2.50 | 0.44 |
| 11:V:47:THR:OG1 | 9:IC:115:ASN:OD1 | 2.34 | 0.44 |
| 11:IE:2:LEU:HD23 | 11:IE:32:TYR:CD1 | 2.53 | 0.44 |
| 5:J:104:VAL:HG22 | 5:J:105:ASN:H | 1.83 | 0.44 |
| 5:J:135:LEU:HA | 5:J:144:GLU:O | 2.18 | 0.44 |
| 5:J:302:GLU:HB3 | 5:J:365:ILE:CD1 | 2.47 | 0.44 |
| 5:J:469:PRO:HA | 5:J:472:TYR:CZ | 2.52 | 0.44 |
| 5:J:58:GLN:OE1 | 5:J:58:GLN:N | 2.42 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:M:69:THR:HA | 6:N:73:ASN:CB | 2.47 | 0.44 |
| 7:O:231:GLY:H | 7:O:243:VAL:HB | 1.81 | 0.44 |
| 7:O:485:ASN:OD1 | 7:Q:448:ALA:N | 2.50 | 0.44 |
| 7:O:59:PHE:HB2 | 7:O:74:LYS:HG2 | 1.99 | 0.44 |
| 7:O:97:LEU:HD22 | 7:P:96:GLY:HA2 | 1.99 | 0.44 |
| 7:Q:26:PRO:HA | 7:Q:27:PRO:HD3 | 1.69 | 0.44 |
| 8:R:69:TRP:CZ3 | 8:R:157:LEU:HD12 | 2.51 | 0.44 |
| 8:R:98:GLU:N | 8:R:98:GLU:OE1 | 2.48 | 0.44 |
| 11:V:14:LYS:O | 11:V:15:THR:HG22 | 2.17 | 0.44 |
| 1:X:236:PHE:N | 1:X:236:PHE:CD1 | 2.84 | 0.44 |
| 1:X:59:LEU:CD1 | 1:Y:37:LEU:HD12 | 2.48 | 0.44 |
| 1:X:7:ASN:OD1 | 1:X:7:ASN:N | 2.50 | 0.44 |
| 1:Y:188:TYR:HD1 | 1:Y:233:ASN:ND2 | 2.15 | 0.44 |
| 1:Y:41:ASN:O | 1:Y:42:GLU:HG2 | 2.18 | 0.44 |
| 1:Y:533:ASP:OD1 | 1:Y:534:VAL:HG22 | 2.18 | 0.44 |
| 13:YA:112[E]:GLU:C | 13:YA:115[E]:SER:HB3 | 2.38 | 0.44 |
| 13:YA:261[F]:LYS:HE2 | 13:YA:293[F]:ASN:HB3 | 1.99 | 0.44 |
| 13:YA:314[E]:SER:OG | 13:YA:316[E]:TRP:HB3 | 2.17 | 0.44 |
| 13:YA:315[E]:LEU:O | 13:YA:319[E]:GLN:HG2 | 2.16 | 0.44 |
| 13:YA:516[A]:GLY:O | 13:YC:522[A]:VAL:HG23 | 2.17 | 0.44 |
| 13:YA:534[F]:LEU:HD11 | 13:YA:536[F]:TRP:NE1 | 2.32 | 0.44 |
| 13:YA:537[A]:LYS:C | 13:YA:537[A]:LYS:HD3 | 2.37 | 0.44 |
| 13:YA:537[B]:LYS:C | 13:YA:537[B]:LYS:HD3 | 2.37 | 0.44 |
| 13:YA:66[A]:MET:HE2 | 13:YB:122[A]:PRO:HB3 | 1.98 | 0.44 |
| 13:YB:109[D]:ASN:OD1 | 13:YB:110[D]:ARG:N | 2.51 | 0.44 |
| 13:YB:252[C]:MET:HB3 | 13:YB:252[C]:MET:HE3 | 1.86 | 0.44 |
| 13:YB:261[C]:LYS:HE2 | 13:YB:293[C]:ASN:HB3 | 1.99 | 0.44 |
| 13:YB:261[E]:LYS:HE2 | 13:YB:293[E]:ASN:HB3 | 1.99 | 0.44 |
| 13:YB:36[D]:PRO:HB2 | 13:YB:38[D]:GLN:OE1 | 2.17 | 0.44 |
| 13:YB:50[F]:GLU:CD | 13:YB:50[F]:GLU:N | 2.71 | 0.44 |
| 13:YA:565[D]:TYR:CZ | 13:YB:557[D]:MET:HG2 | 2.53 | 0.44 |
| 13:YB:67[F]:SER:HB3 | 13:YC:123[F]:ARG:HB2 | 1.99 | 0.44 |
| 13:YC:109[D]:ASN:OD1 | 13:YC:110[D]:ARG:N | 2.51 | 0.44 |
| 13:YC:110[F]:ARG:HD2 | 13:YC:118[F]:THR:O | 2.17 | 0.44 |
| 13:YC:109[A]:ASN:OD1 | 13:YC:110[A]:ARG:N | 2.51 | 0.44 |
| 13:YC:147[C]:ILE:HD11 | 13:YC:188[C]:LEU:HG | 2.00 | 0.44 |
| 13:YC:236[D]:ILE:HG23 | 13:YC:240[D]:GLU:HB2 | 2.00 | 0.44 |
| 13:YA:438[E]:LEU:CD2 | 13:YC:442[E]:THR:HG21 | 2.48 | 0.44 |
| 13:YA:516[F]:GLY:O | 13:YC:522[F]:VAL:HG23 | 2.17 | 0.44 |
| 13:YC:537[D]:LYS:C | 13:YC:537[D]:LYS:HD3 | 2.37 | 0.44 |
| 14:YD:288[D]:TYR:CE1 | 14:YD:371[D]:LYS:HD3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:140[E]:TYR:HE2 | 14:YE:148[E]:PRO:HD3 | 1.82 | 0.44 |
| 14:YE:135[C]:MET:SD | 14:YE:166[C]:PHE:HD1 | 2.40 | 0.44 |
| 14:YE:233[A]:ASP:N | 14:YE:233[A]:ASP:OD1 | 2.51 | 0.44 |
| 14:YE:233[E]:ASP:N | 14:YE:233[E]:ASP:OD1 | 2.51 | 0.44 |
| 14:YE:307[B]:TYR:HD1 | 14:YE:307[B]:TYR:HA | 1.66 | 0.44 |
| 14:YE:307[D]:TYR:HA | 14:YE:307[D]:TYR:HD1 | 1.66 | 0.44 |
| 14:YE:88[D]:TYR:HD1 | 14:YE:110[D]:GLY:C | 2.21 | 0.44 |
| 14:YF:127[D]:ASP:CG | 14:YF:130[D]:GLU:H | 2.19 | 0.44 |
| 14:YF:135[A]:MET:SD | 14:YF:166[A]:PHE:HD1 | 2.40 | 0.44 |
| 14:YF:233[E]:ASP:OD1 | 14:YF:233[E]:ASP:N | 2.51 | 0.44 |
| 2:Z:191:TYR:HE2 | 2:Z:204:ARG:HB3 | 1.82 | 0.44 |
| 1:A:178:ILE:HA | 1:A:178:ILE:HD12 | 1.84 | 0.44 |
| 1:A:210:THR:CG2 | 1:A:226:MET:H | 2.31 | 0.44 |
| 1:A:200:TYR:HB2 | 1:A:269:VAL:HG13 | 1.98 | 0.44 |
| 1:A:288:TYR:CE2 | 1:A:290:ASP:O | 2.70 | 0.44 |
| 1:A:365:ASP:OD2 | 1:A:367:THR:HB | 2.18 | 0.44 |
| 1:A:413:TYR:CE1 | 1:A:415:PHE:HE1 | 2.36 | 0.44 |
| 1:A:52:ARG:HD3 | 9:T:22:ASP:OD2 | 2.17 | 0.44 |
| 1:A:619:GLN:CD | 1:A:619:GLN:H | 2.18 | 0.44 |
| 5:AC:135:LEU:HA | 5:AC:144:GLU:O | 2.17 | 0.44 |
| 5:AC:184:THR:H | 5:AC:307:ASN:ND2 | 2.13 | 0.44 |
| 5:AC:267:ASP:CG | 5:AC:285:LEU:HB2 | 2.38 | 0.44 |
| 5:AC:323:THR:HG21 | 5:AC:354:THR:HG23 | 1.98 | 0.44 |
| 5:AC:408:VAL:HG23 | 5:AE:409:SER:O | 2.18 | 0.44 |
| 5:AD:551:ILE:HD13 | 5:AE:565:ILE:CD1 | 2.46 | 0.44 |
| 5:AD:597:ARG:HH12 | 5:AE:489:GLY:N | 2.16 | 0.44 |
| 5:AE:131:SER:HA | 5:AE:150:GLN:HA | 1.99 | 0.44 |
| 5:AE:477:SER:N | 5:AE:602:ALA:O | 2.28 | 0.44 |
| 6:AF:87:TYR:N | 6:AF:181:GLU:O | 2.32 | 0.44 |
| 6:AH:203:LEU:HD12 | 6:AH:206:GLN:NE2 | 2.31 | 0.44 |
| 7:AI:262:VAL:HB | 7:AJ:261:GLY:N | 2.33 | 0.44 |
| 7:AI:288:ILE:HG13 | 7:BA:288:ILE:HG22 | 2.00 | 0.44 |
| 7:BA:161:THR:H | 7:BA:164:LYS:HB2 | 1.83 | 0.44 |
| 8:BC:32:PHE:O | 8:BC:35:GLN:N | 2.50 | 0.44 |
| 12:BG:16:PHE:CB | 12:DJ:236:ILE:HD11 | 2.48 | 0.44 |
| 1:BH:270:ILE:HD13 | 1:BH:270:ILE:HG21 | 1.69 | 0.44 |
| 1:BH:440:ILE:HG13 | 1:BH:441:ILE:N | 2.31 | 0.44 |
| 1:BH:557:PRO:HB3 | 1:BH:589:TYR:CZ | 2.53 | 0.44 |
| 2:BJ:160:VAL:O | 2:BJ:163:ILE:HB | 2.18 | 0.44 |
| 2:BJ:796:THR:HG23 | 2:BJ:797:TYR:CD2 | 2.52 | 0.44 |
| 2:BJ:921:TRP:CD1 | 2:BJ:921:TRP:N | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1005:ARG:NH1 | 5:I:12:ASP:OD2 | 2.50 | 0.44 |
| 2:C:138:ASN:O | 2:C:555:ARG:CZ | 2.64 | 0.44 |
| 2:C:251:ASP:CG | 2:C:252:LYS:HG3 | 2.38 | 0.44 |
| 5:CF:355:ASP:OD1 | 5:CF:356:TYR:N | 2.49 | 0.44 |
| 5:CG:135:LEU:HA | 5:CG:144:GLU:O | 2.18 | 0.44 |
| 5:CG:597:ARG:HH12 | 5:CH:489:GLY:N | 2.16 | 0.44 |
| 6:CJ:73:ASN:ND2 | 6:CJ:215:PHE:HE2 | 2.16 | 0.44 |
| 3:D:232:GLN:N | 3:D:232:GLN:OE1 | 2.42 | 0.44 |
| 6:DA:13:ARG:HG2 | 6:DA:14:LEU:N | 2.27 | 0.44 |
| 6:DA:195:LEU:HD13 | 6:DA:215:PHE:CE1 | 2.52 | 0.44 |
| 7:DB:77:THR:HG22 | 7:DB:80:THR:H | 1.83 | 0.44 |
| 7:DB:476:ASP:N | 7:DC:470:GLY:O | 2.40 | 0.44 |
| 7:DB:327:GLN:HG3 | 7:DD:322:THR:O | 2.17 | 0.44 |
| 1:BH:52:ARG:HD3 | 9:DG:22:ASP:OD2 | 2.17 | 0.44 |
| 9:DG:96:ILE:O | 9:DG:105:ILE:HG22 | 2.17 | 0.44 |
| 11:DI:88:THR:HG22 | 11:DI:92:ALA:HB3 | 1.99 | 0.44 |
| 3:E:197:ASP:OD1 | 3:E:198:VAL:N | 2.48 | 0.44 |
| 1:EA:123:ILE:HD11 | 1:EA:295:ILE:HD11 | 2.00 | 0.44 |
| 1:EA:277:GLY:O | 1:EA:279:ASP:N | 2.50 | 0.44 |
| 1:EA:432:SER:O | 1:EA:435:TRP:HB3 | 2.18 | 0.44 |
| 1:EB:330:THR:HG23 | 1:EB:333:ARG:HE | 1.83 | 0.44 |
| 1:EB:491:PHE:HE2 | 1:EB:619:GLN:HA | 1.82 | 0.44 |
| 1:EB:486:ARG:NH2 | 1:EB:500:LYS:O | 2.51 | 0.44 |
| 2:EC:737:THR:HB | 2:EC:740:ILE:HD12 | 1.98 | 0.44 |
| 2:EC:821:ILE:O | 2:EC:824:GLN:NE2 | 2.32 | 0.44 |
| 2:EC:711:ARG:HD3 | 2:EC:878:ASP:OD1 | 2.18 | 0.44 |
| 3:ED:64:SER:HG | 3:ED:67:GLY:H | 1.58 | 0.44 |
| 3:ED:72:TRP:CE2 | 3:ED:305:HIS:HA | 2.53 | 0.44 |
| 2:BJ:528:ASN:HB3 | 3:EE:233:GLN:NE2 | 2.33 | 0.44 |
| 4:EH:107:VAL:O | 4:EH:148:LEU:N | 2.39 | 0.44 |
| 5:EI:275:SER:HA | 5:EI:280:ILE:HG22 | 2.00 | 0.44 |
| 5:EJ:469:PRO:HA | 5:EJ:472:TYR:CZ | 2.52 | 0.44 |
| 5:FA:320:LEU:HG | 5:FA:357:SER:HB3 | 2.00 | 0.44 |
| 5:EJ:410:GLN:N | 5:FA:406:LEU:O | 2.25 | 0.44 |
| 5:FA:58:GLN:OE1 | 5:FA:58:GLN:N | 2.37 | 0.44 |
| 5:FA:84:GLY:C | 5:FA:86:VAL:H | 2.17 | 0.44 |
| 6:FD:73:ASN:ND2 | 6:FD:215:PHE:HE2 | 2.16 | 0.44 |
| 7:FE:262:VAL:HB | 7:FF:261:GLY:N | 2.31 | 0.44 |
| 7:FF:198:GLN:HA | 7:FF:201:GLN:CD | 2.38 | 0.44 |
| 7:FE:327:GLN:HG3 | 7:FG:322:THR:O | 2.17 | 0.44 |
| 7:FE:401:ARG:NH2 | 7:FG:397:GLY:O | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FG:67:ILE:HA | 7:FG:84:ARG:NH2 | 2.31 | 0.44 |
| 7:FG:77:THR:HG22 | 7:FG:80:THR:H | 1.82 | 0.44 |
| 8:DF:41:LEU:HD22 | 8:FI:140:LEU:HD23 | 1.98 | 0.44 |
| 10:GA:221:ALA:O | 10:GA:224:ASN:HB3 | 2.16 | 0.44 |
| 11:GB:2:LEU:HD23 | 11:GB:32:TYR:CD1 | 2.53 | 0.44 |
| 12:DJ:16:PHE:CB | 12:GC:236:ILE:HD11 | 2.48 | 0.44 |
| 1:GE:188:TYR:HD1 | 1:GE:233:ASN:ND2 | 2.15 | 0.44 |
| 1:GE:486:ARG:NH2 | 1:GE:500:LYS:O | 2.51 | 0.44 |
| 2:GF:168:ILE:CG2 | 2:GF:169:GLY:N | 2.81 | 0.44 |
| 2:GF:251:ASP:CG | 2:GF:252:LYS:HG3 | 2.38 | 0.44 |
| 3:GG:147:LEU:HD11 | 3:GG:152:GLU:CD | 2.37 | 0.44 |
| 3:GG:249:PHE:O | 3:GG:329:ASN:HA | 2.16 | 0.44 |
| 3:GG:64:SER:HG | 3:GG:67:GLY:H | 1.60 | 0.44 |
| 4:GJ:68:GLN:HB3 | 4:GJ:70:HIS:NE2 | 2.32 | 0.44 |
| 4:H:192:PHE:CE1 | 4:H:197:TYR:HB2 | 2.53 | 0.44 |
| 4:HA:145:LYS:N | 4:HA:165:GLU:O | 2.49 | 0.44 |
| 5:HB:267:ASP:CG | 5:HB:285:LEU:HB2 | 2.38 | 0.44 |
| 5:HB:321:ALA:HA | 5:HB:358:VAL:CB | 2.44 | 0.44 |
| 5:HB:85:THR:HB | 5:HB:137:TYR:CE2 | 2.52 | 0.44 |
| 5:HB:317:LEU:HD13 | 5:HC:312:ARG:HH12 | 1.83 | 0.44 |
| 5:HD:102:TRP:CD1 | 5:HD:102:TRP:N | 2.83 | 0.44 |
| 5:HD:293:PHE:HZ | 5:HD:366:PRO:O | 2.00 | 0.44 |
| 5:HD:393:LEU:O | 5:HD:394:LEU:HB2 | 2.16 | 0.44 |
| 6:HF:91:SER:OG | 6:HF:177:THR:HB | 2.18 | 0.44 |
| 7:HH:283:TRP:CZ3 | 7:HH:284:ASN:HB3 | 2.52 | 0.44 |
| 5:HB:239:GLY:O | 7:HH:2:SER:N | 2.51 | 0.44 |
| 7:HH:301:ARG:O | 7:HJ:295:ILE:HA | 2.17 | 0.44 |
| 7:HH:32:VAL:O | 7:HH:36:ILE:HG12 | 2.18 | 0.44 |
| 7:HH:59:PHE:HB2 | 7:HH:74:LYS:HG2 | 1.99 | 0.44 |
| 7:HI:232:THR:HG22 | 7:HI:235:GLU:HG3 | 2.00 | 0.44 |
| 7:HJ:493:GLU:HA | 7:HJ:496:ARG:NH2 | 2.32 | 0.44 |
| 5:I:196:ARG:HH11 | 7:O:5:THR:CG2 | 2.28 | 0.44 |
| 5:I:275:SER:HA | 5:I:280:ILE:HG22 | 2.00 | 0.44 |
| 8:IB:69:TRP:CZ3 | 8:IB:157:LEU:HD12 | 2.51 | 0.44 |
| 8:IA:6:VAL:HB | 8:IB:53:PHE:CD1 | 2.52 | 0.44 |
| 11:IE:14:LYS:O | 11:IE:15:THR:HG22 | 2.17 | 0.44 |
| 5:J:466:PRO:HA | 5:J:596:TYR:CZ | 2.52 | 0.44 |
| 5:K:265:LEU:HB3 | 5:K:281:TYR:HB3 | 1.99 | 0.44 |
| 5:K:326:MET:HE3 | 5:K:326:MET:HB2 | 1.67 | 0.44 |
| 5:I:264:ARG:NH2 | 6:M:3:LEU:HD13 | 2.33 | 0.44 |
| 7:O:260:ARG:HD3 | 7:Q:262:VAL:HG23 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:329:ASN:OD1 | 7:O:330:ARG:N | 2.50 | 0.44 |
| 7:O:87:TYR:HB3 | 7:O:88:PRO:HD3 | 1.99 | 0.44 |
| 7:P:129:PHE:CE2 | 7:P:141:VAL:HG11 | 2.52 | 0.44 |
| 7:O:161:THR:HA | 7:P:158:THR:O | 2.17 | 0.44 |
| 1:X:595:ILE:HG21 | 1:X:602:ILE:HG23 | 2.00 | 0.44 |
| 1:Y:451:ASP:O | 1:Y:454:ILE:HD12 | 2.17 | 0.44 |
| 13:YA:147[B]:ILE:HD11 | 13:YA:188[B]:LEU:HG | 2.00 | 0.44 |
| 13:YA:516[C]:GLY:O | 13:YC:522[C]:VAL:HG23 | 2.17 | 0.44 |
| 13:YA:534[C]:LEU:HD11 | 13:YA:536[C]:TRP:NE1 | 2.32 | 0.44 |
| 13:YA:558[B]:SER:N | 13:YB:550[B]:TRP:O | 2.50 | 0.44 |
| 13:YB:110[C]:ARG:HD2 | 13:YB:118[C]:THR:O | 2.17 | 0.44 |
| 13:YB:257[C]:LYS:HE2 | 13:YB:266[C]:TRP:CH2 | 2.52 | 0.44 |
| 13:YB:336[D]:LEU:HA | 13:YB:336[D]:LEU:HD12 | 1.85 | 0.44 |
| 13:YA:376[B]:PHE:CD2 | 13:YB:447[B]:ASN:OD1 | 2.71 | 0.44 |
| 13:YB:540[E]:GLY:HA3 | 13:YC:533[E]:ASN:ND2 | 2.22 | 0.44 |
| 13:YA:7[D]:ASN:ND2 | 13:YB:9[D]:ASN:HA | 2.21 | 0.44 |
| 13:YC:261[A]:LYS:HE2 | 13:YC:293[A]:ASN:HB3 | 1.99 | 0.44 |
| 13:YC:257[E]:LYS:HE2 | 13:YC:266[E]:TRP:CH2 | 2.53 | 0.44 |
| 13:YC:315[A]:LEU:O | 13:YC:319[A]:GLN:HG2 | 2.16 | 0.44 |
| 13:YC:36[A]:PRO:HB2 | 13:YC:38[A]:GLN:OE1 | 2.17 | 0.44 |
| 13:YA:543[B]:ASP:HA | 13:YC:551[B]:THR:O | 2.17 | 0.44 |
| 13:YC:552[A]:GLU:CG | 13:YC:554[A]:MET:HE1 | 2.47 | 0.44 |
| 13:YA:394[D]:GLU:N | 13:YC:70[D]:GLY:O | 2.50 | 0.44 |
| 14:YD:109[D]:LEU:HD12 | 14:YD:109[D]:LEU:HA | 1.65 | 0.44 |
| 14:YD:135[E]:MET:SD | 14:YD:166[E]:PHE:HD1 | 2.40 | 0.44 |
| 14:YD:236[B]:TRP:N | 14:YE:95[B]:VAL:O | 2.51 | 0.44 |
| 14:YD:288[F]:TYR:CE1 | 14:YD:371[F]:LYS:HD3 | 2.52 | 0.44 |
| 14:YD:38[D]:LEU:HD12 | 14:YD:38[D]:LEU:HA | 1.63 | 0.44 |
| 14:YE:140[C]:TYR:HE2 | 14:YE:148[C]:PRO:HD3 | 1.82 | 0.44 |
| 14:YE:140[D]:TYR:HE2 | 14:YE:148[D]:PRO:HD3 | 1.82 | 0.44 |
| 11:V:190:LYS:NZ | 14:YE:24[F]:SER:HA | 2.33 | 0.44 |
| 13:YB:92[B]:THR:HB | 14:YE:282[B]:ALA:CB | 2.48 | 0.44 |
| 14:YE:288[A]:TYR:CE1 | 14:YE:371[A]:LYS:HD3 | 2.52 | 0.44 |
| 14:YE:277[A]:VAL:HG11 | 14:YE:294[A]:GLU:HG2 | 1.99 | 0.44 |
| 14:YE:73[F]:SER:HB2 | 14:YE:85[F]:THR:HG23 | 1.99 | 0.44 |
| 14:YF:140[F]:TYR:HE2 | 14:YF:148[F]:PRO:HD3 | 1.82 | 0.44 |
| 14:YF:288[C]:TYR:CE1 | 14:YF:371[C]:LYS:HD3 | 2.53 | 0.44 |
| 14:YF:73[A]:SER:HA | 14:YF:85[A]:THR:HA | 1.99 | 0.44 |
| 14:YF:73[F]:SER:HA | 14:YF:85[F]:THR:HA | 1.99 | 0.44 |
| 2:Z:251:ASP:CG | 2:Z:252:LYS:HG3 | 2.38 | 0.44 |
| 2:Z:400:ASP:O | 2:Z:424:ARG:NH1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:613:LYS:O | 2:Z:615:THR:N | 2.47 | 0.44 |
| 2:Z:855:ILE:HA | 2:Z:855:ILE:HD12 | 1.86 | 0.44 |
| 1:A:384:LEU:HA | 1:A:384:LEU:HD23 | 1.83 | 0.44 |
| 1:A:595:ILE:CG2 | 1:A:602:ILE:HG23 | 2.47 | 0.44 |
| 5:AD:323:THR:HB | 5:AD:355:ASP:HB3 | 1.99 | 0.44 |
| 5:AD:80:ASN:C | 5:AD:81:LEU:HD12 | 2.38 | 0.44 |
| 6:AH:13:ARG:HG2 | 6:AH:14:LEU:N | 2.27 | 0.44 |
| 7:AI:463:THR:HG23 | 7:BA:483:PHE:HE1 | 1.82 | 0.44 |
| 7:AI:59:PHE:HB2 | 7:AI:74:LYS:HG2 | 1.99 | 0.44 |
| 7:AJ:360:ARG:HH11 | 7:AJ:525:VAL:HG21 | 1.80 | 0.44 |
| 1:B:332:LYS:O | 1:B:335:THR:HG22 | 2.18 | 0.44 |
| 9:BD:58:SER:O | 9:BD:62:PHE:N | 2.34 | 0.44 |
| 1:BH:339:CYS:SG | 1:BH:400:ASN:HA | 2.57 | 0.44 |
| 1:BH:7:ASN:OD1 | 1:BH:7:ASN:N | 2.50 | 0.44 |
| 2:BJ:425:ARG:NH2 | 2:BJ:447:ASN:HD21 | 2.15 | 0.44 |
| 2:BJ:479:TRP:HE3 | 2:BJ:479:TRP:H | 1.64 | 0.44 |
| 2:BJ:584:GLY:HA2 | 2:BJ:600:PHE:CB | 2.46 | 0.44 |
| 2:BJ:724:ALA:C | 2:BJ:726:PHE:H | 2.20 | 0.44 |
| 2:C:612:TRP:CD1 | 2:C:618:PHE:HB3 | 2.53 | 0.44 |
| 2:C:796:THR:HG23 | 2:C:797:TYR:CD2 | 2.52 | 0.44 |
| 2:C:975:ASN:OD1 | 2:C:981:GLN:HB3 | 2.16 | 0.44 |
| 3:CA:128:TRP:HB2 | 3:CA:194:ILE:HB | 1.99 | 0.44 |
| 3:CA:130:VAL:HG21 | 3:CA:192:PHE:CZ | 2.53 | 0.44 |
| 3:CA:150:LYS:HE2 | 3:CA:160:TRP:CD1 | 2.53 | 0.44 |
| 3:CB:79:VAL:HG12 | 3:CB:80:LYS:O | 2.18 | 0.44 |
| 4:CC:192:PHE:CE1 | 4:CC:197:TYR:HB2 | 2.53 | 0.44 |
| 5:CF:522:SER:C | 5:CH:591:PRO:HD3 | 2.38 | 0.44 |
| 5:CG:115:ASP:OD2 | 5:CG:137:TYR:HE1 | 2.01 | 0.44 |
| 5:CG:304:ILE:CD1 | 5:CG:385:TRP:HA | 2.40 | 0.44 |
| 5:CG:480:LEU:HD23 | 5:CG:480:LEU:HA | 1.81 | 0.44 |
| 5:CH:290:SER:HB3 | 5:CH:371:PHE:N | 2.32 | 0.44 |
| 5:CF:549:SER:N | 5:CH:569:TYR:O | 2.51 | 0.44 |
| 6:CJ:71:ILE:O | 6:CJ:215:PHE:N | 2.36 | 0.44 |
| 7:DC:360:ARG:HH11 | 7:DC:525:VAL:HG21 | 1.80 | 0.44 |
| 7:DD:133:VAL:HA | 7:DD:141:VAL:O | 2.18 | 0.44 |
| 7:DD:228:ILE:HG22 | 7:DD:229:LYS:N | 2.33 | 0.44 |
| 7:DB:504:ARG:NH2 | 7:DD:424:ARG:O | 2.48 | 0.44 |
| 7:DD:88:PRO:HG2 | 7:DD:95:TYR:O | 2.16 | 0.44 |
| 8:DF:22:GLN:OE1 | 8:DF:116:TYR:OH | 2.25 | 0.44 |
| 9:DG:33:LYS:HG2 | 9:DG:122:ILE:HG21 | 1.99 | 0.44 |
| 1:EA:278:ALA:HB2 | 1:EA:317:GLY:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:595:ILE:CG2 | 1:EA:602:ILE:HG23 | 2.47 | 0.44 |
| 1:EB:41:ASN:O | 1:EB:42:GLU:HG2 | 2.18 | 0.44 |
| 2:EC:380:ILE:O | 2:EC:401:LYS:HA | 2.17 | 0.44 |
| 2:EC:748:PHE:CD2 | 2:EC:756:VAL:HG11 | 2.52 | 0.44 |
| 3:ED:274:ILE:HD12 | 3:ED:311:TYR:HB3 | 1.99 | 0.44 |
| 4:EF:168:PHE:CE1 | 4:EG:149:ARG:HB3 | 2.53 | 0.44 |
| 5:EI:104:VAL:HG13 | 5:EI:105:ASN:H | 1.83 | 0.44 |
| 5:EI:214:SER:HB2 | 5:EI:215:PRO:HD2 | 1.98 | 0.44 |
| 5:EI:317:LEU:HD13 | 5:EJ:312:ARG:NH1 | 2.32 | 0.44 |
| 5:EJ:323:THR:HG22 | 5:EJ:355:ASP:O | 2.18 | 0.44 |
| 5:EJ:361:ASP:H | 5:EJ:366:PRO:HB3 | 1.82 | 0.44 |
| 5:EJ:34:TYR:OH | 5:EJ:42:VAL:N | 2.50 | 0.44 |
| 5:EJ:503:ASN:OD1 | 5:EJ:504:ASN:N | 2.49 | 0.44 |
| 4:F:111:ASN:HB2 | 4:F:116:ILE:HD12 | 1.98 | 0.44 |
| 4:F:1:MET:HG2 | 4:F:70:HIS:ND1 | 2.32 | 0.44 |
| 7:FE:283:TRP:CZ3 | 7:FE:284:ASN:HB3 | 2.52 | 0.44 |
| 7:FF:13:SER:HB2 | 7:FG:18:PHE:HA | 2.00 | 0.44 |
| 7:FG:228:ILE:HG22 | 7:FG:229:LYS:N | 2.33 | 0.44 |
| 7:FG:240:ASN:HB3 | 7:FG:243:VAL:HG22 | 2.00 | 0.44 |
| 7:FG:63:GLU:O | 7:FG:67:ILE:HG12 | 2.16 | 0.44 |
| 1:EA:69:GLN:HE21 | 11:GB:25:MET:HE1 | 1.82 | 0.44 |
| 1:GD:595:ILE:CG2 | 1:GD:602:ILE:HG23 | 2.47 | 0.44 |
| 2:GF:193:MET:HB3 | 2:GF:200:TYR:HB2 | 1.98 | 0.44 |
| 2:GF:562:ASP:O | 2:GF:565:ASP:N | 2.44 | 0.44 |
| 2:GF:725:ARG:HA | 2:GF:728:GLU:HB3 | 2.00 | 0.44 |
| 3:GG:150:LYS:HE2 | 3:GG:160:TRP:CD1 | 2.53 | 0.44 |
| 2:GF:915:LYS:HG2 | 3:GG:326:GLU:OE2 | 2.18 | 0.44 |
| 3:GG:72:TRP:CE2 | 3:GG:305:HIS:HA | 2.53 | 0.44 |
| 3:GG:86:LEU:HA | 3:GG:86:LEU:HD23 | 1.68 | 0.44 |
| 3:GH:178:GLY:O | 3:GH:180:ILE:N | 2.51 | 0.44 |
| 4:GJ:152:SER:O | 4:GJ:158:SER:HA | 2.18 | 0.44 |
| 4:HA:152:SER:O | 4:HA:158:SER:HA | 2.18 | 0.44 |
| 5:HB:150:GLN:HG3 | 5:HB:151:ILE:O | 2.18 | 0.44 |
| 5:HC:285:LEU:HD21 | 5:HC:375:PHE:N | 2.21 | 0.44 |
| 5:HC:7:ILE:HD11 | 5:HD:24:ILE:HD11 | 1.99 | 0.44 |
| 7:HH:111:ASN:CG | 7:HH:114:SER:HB3 | 2.38 | 0.44 |
| 7:HH:288:ILE:HG13 | 7:HJ:288:ILE:HG22 | 2.00 | 0.44 |
| 7:HI:99:ARG:HG2 | 7:HI:100:TYR:O | 2.17 | 0.44 |
| 7:HI:110:VAL:HG12 | 7:HI:111:ASN:N | 2.32 | 0.44 |
| 7:HI:77:THR:HA | 7:HJ:74:LYS:O | 2.17 | 0.44 |
| 7:HJ:125:LEU:O | 7:HJ:129:PHE:N | 2.40 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:153:LYS:HE3 | 5:I:155:THR:OG1 | 2.17 | 0.44 |
| 5:I:317:LEU:HD13 | 5:J:312:ARG:HH12 | 1.82 | 0.44 |
| 5:I:402:GLU:HG2 | 5:K:396:LYS:HE3 | 2.00 | 0.44 |
| 5:I:402:GLU:HG3 | 5:I:406:LEU:CD1 | 2.47 | 0.44 |
| 9:IC:10:ASP:O | 9:IC:26:SER:N | 2.48 | 0.44 |
| 10:ID:203:ARG:NH1 | 10:ID:311:PHE:HE1 | 2.16 | 0.44 |
| 8:IA:53:PHE:HB2 | 12:IF:7:PHE:CE2 | 2.52 | 0.44 |
| 5:K:176:ASP:HA | 5:K:231:ARG:HA | 1.99 | 0.44 |
| 6:L:13:ARG:HG2 | 6:L:14:LEU:N | 2.27 | 0.44 |
| 6:L:91:SER:OG | 6:L:177:THR:HB | 2.18 | 0.44 |
| 6:N:195:LEU:HD13 | 6:N:215:PHE:CE1 | 2.52 | 0.44 |
| 7:O:349:TRP:NE1 | 7:O:353:SER:O | 2.50 | 0.44 |
| 7:O:262:VAL:HB | 7:P:261:GLY:N | 2.33 | 0.44 |
| 7:P:418:ASP:HA | 7:P:424:ARG:NH2 | 2.31 | 0.44 |
| 7:P:445:HIS:CE1 | 7:Q:447:HIS:CE1 | 3.06 | 0.44 |
| 7:Q:77:THR:HG22 | 7:Q:80:THR:H | 1.82 | 0.44 |
| 8:R:118:ARG:NH2 | 8:S:62:GLY:O | 2.51 | 0.44 |
| 1:X:209:TRP:CD1 | 1:X:225:TYR:HE1 | 2.34 | 0.44 |
| 1:Y:206:TRP:CE2 | 1:Y:222:THR:HB | 2.52 | 0.44 |
| 1:Y:423:THR:O | 1:Y:476:ILE:N | 2.45 | 0.44 |
| 13:YA:147[A]:ILE:HD11 | 13:YA:188[A]:LEU:HG | 2.00 | 0.44 |
| 13:YA:257[F]:LYS:HE2 | 13:YA:266[F]:TRP:CH2 | 2.52 | 0.44 |
| 13:YA:263[D]:GLY:N | 13:YA:264[D]:PRO:HD2 | 2.33 | 0.44 |
| 13:YA:257[B]:LYS:HE2 | 13:YA:266[B]:TRP:CH2 | 2.53 | 0.44 |
| 13:YA:36[C]:PRO:HB2 | 13:YA:38[C]:GLN:OE1 | 2.17 | 0.44 |
| 13:YA:552[F]:GLU:CG | 13:YA:554[F]:MET:HE1 | 2.47 | 0.44 |
| 13:YA:558[C]:SER:N | 13:YB:550[C]:TRP:O | 2.50 | 0.44 |
| 13:YB:112[E]:GLU:C | 13:YB:115[E]:SER:HB3 | 2.38 | 0.44 |
| 13:YB:110[B]:ARG:HD2 | 13:YB:118[B]:THR:O | 2.17 | 0.44 |
| 13:YB:236[E]:ILE:HG23 | 13:YB:240[E]:GLU:HB2 | 1.99 | 0.44 |
| 13:YB:257[B]:LYS:HE2 | 13:YB:266[B]:TRP:CH2 | 2.53 | 0.44 |
| 13:YB:314[B]:SER:OG | 13:YB:316[B]:TRP:HB3 | 2.17 | 0.44 |
| 13:YB:314[C]:SER:OG | 13:YB:316[C]:TRP:HB3 | 2.18 | 0.44 |
| 13:YB:36[C]:PRO:HB2 | 13:YB:38[C]:GLN:OE1 | 2.17 | 0.44 |
| 13:YB:490[D]:VAL:HG12 | 13:YB:492[D]:GLY:H | 1.82 | 0.44 |
| 13:YB:537[A]:LYS:C | 13:YB:537[A]:LYS:HD3 | 2.37 | 0.44 |
| 13:YB:66[D]:MET:HA | 13:YB:66[D]:MET:HE3 | 1.99 | 0.44 |
| 13:YA:473[E]:GLN:OE1 | 13:YC:158[E]:PRO:HB2 | 2.18 | 0.44 |
| 13:YC:236[E]:ILE:HG23 | 13:YC:240[E]:GLU:HB2 | 1.99 | 0.44 |
| 13:YC:314[A]:SER:OG | 13:YC:316[A]:TRP:HB3 | 2.17 | 0.44 |
| 13:YA:450[C]:VAL:O | 13:YC:459[C]:GLY:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:551[B]:THR:HA | 13:YC:558[B]:SER:O | 2.18 | 0.44 |
| 13:YA:551[F]:THR:HA | 13:YC:558[F]:SER:O | 2.18 | 0.44 |
| 14:YD:234[B]:PHE:HD1 | 14:YE:97[B]:VAL:HG12 | 1.83 | 0.44 |
| 14:YD:277[D]:VAL:HG11 | 14:YD:294[D]:GLU:HG2 | 1.98 | 0.44 |
| 14:YD:364[E]:LEU:HA | 14:YD:364[E]:LEU:HD22 | 1.79 | 0.44 |
| 14:YD:288[B]:TYR:CE1 | 14:YD:371[B]:LYS:HD3 | 2.52 | 0.44 |
| 14:YD:44[C]:LEU:HB2 | 14:YD:340[C]:ASP:O | 2.18 | 0.44 |
| 14:YD:95[F]:VAL:O | 14:YF:236[F]:TRP:N | 2.51 | 0.44 |
| 14:YE:127[D]:ASP:CG | 14:YE:130[D]:GLU:H | 2.20 | 0.44 |
| 14:YE:233[F]:ASP:OD1 | 14:YE:233[F]:ASP:N | 2.51 | 0.44 |
| 13:YB:26[A]:ARG:HD3 | 14:YE:259[A]:LEU:CD2 | 2.48 | 0.44 |
| 14:YE:277[D]:VAL:HG11 | 14:YE:294[D]:GLU:HG2 | 1.98 | 0.44 |
| 14:YE:73[E]:SER:HB2 | 14:YE:85[E]:THR:HG23 | 1.99 | 0.44 |
| 14:YE:73[B]:SER:HA | 14:YE:85[B]:THR:HA | 1.99 | 0.44 |
| 14:YE:86[D]:ARG:HD2 | 14:YE:192[D]:ILE:HD12 | 2.00 | 0.44 |
| 14:YF:140[B]:TYR:HE2 | 14:YF:148[B]:PRO:HD3 | 1.83 | 0.44 |
| 13:YA:81[B]:ARG:HD3 | 14:YF:261[B]:SER:HA | 2.00 | 0.44 |
| 14:YF:279[B]:ARG:HD3 | 14:YF:279[B]:ARG:HA | 1.43 | 0.44 |
| 14:YF:277[F]:VAL:HG11 | 14:YF:294[F]:GLU:HG2 | 1.99 | 0.44 |
| 2:Z:543:LYS:HG2 | 2:Z:575:PHE:CE1 | 2.52 | 0.44 |
| 2:Z:675:LEU:HD12 | 2:Z:675:LEU:HA | 1.67 | 0.44 |
| 2:Z:819:ARG:O | 2:Z:820:LEU:HD23 | 2.17 | 0.44 |
| 15:ZA:26[D]:GLN:NE2 | 15:ZA:29[D]:VAL:H | 1.92 | 0.44 |
| 1:A:123:ILE:HD11 | 1:A:295:ILE:HD11 | 2.00 | 0.44 |
| 1:A:209:TRP:CD1 | 1:A:225:TYR:HE1 | 2.34 | 0.44 |
| 1:A:34:ILE:HG23 | 1:A:48:PHE:CD2 | 2.49 | 0.44 |
| 1:A:81:ARG:HA | 1:A:326:ARG:HG3 | 1.99 | 0.44 |
| 5:AC:290:SER:CA | 5:AC:371:PHE:H | 2.30 | 0.44 |
| 5:AC:418:GLY:C | 5:AE:472:TYR:HB3 | 2.37 | 0.44 |
| 5:AC:522:SER:C | 5:AE:591:PRO:HD3 | 2.38 | 0.44 |
| 5:AD:104:VAL:HG22 | 5:AD:105:ASN:H | 1.83 | 0.44 |
| 6:AF:86:ASP:CG | 6:AF:180:GLN:HE21 | 2.19 | 0.44 |
| 6:AH:130:ARG:O | 6:AH:134:GLN:HG3 | 2.18 | 0.44 |
| 7:AI:167:GLN:O | 7:AI:171:LYS:HG2 | 2.18 | 0.44 |
| 7:AI:260:ARG:HD3 | 7:BA:262:VAL:HG23 | 2.00 | 0.44 |
| 7:AI:77:THR:HG22 | 7:AI:80:THR:H | 1.83 | 0.44 |
| 7:AI:312:GLY:N | 7:AJ:316:THR:O | 2.39 | 0.44 |
| 7:AJ:342:PRO:HB2 | 7:AJ:378:ARG:HH12 | 1.83 | 0.44 |
| 7:AI:97:LEU:HD22 | 7:AJ:96:GLY:HA2 | 2.00 | 0.44 |
| 1:B:276:ASN:HB2 | 1:B:279:ASP:OD2 | 2.18 | 0.44 |
| 7:BA:272:GLN:NE2 | 7:BA:277:ALA:HA | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:504:ARG:NH2 | 7:BA:424:ARG:O | 2.47 | 0.44 |
| 8:BB:14:ASP:CG | 8:BB:17:ARG:HH22 | 2.18 | 0.44 |
| 12:BG:99:SER:HB3 | 12:BG:102:GLY:O | 2.17 | 0.44 |
| 1:BH:210:THR:CG2 | 1:BH:226:MET:H | 2.31 | 0.44 |
| 1:BH:413:TYR:CE1 | 1:BH:415:PHE:HE1 | 2.36 | 0.44 |
| 1:BH:432:SER:O | 1:BH:435:TRP:HB3 | 2.18 | 0.44 |
| 1:BI:205:GLU:C | 1:BI:206:TRP:HD1 | 2.21 | 0.44 |
| 1:BI:533:ASP:OD1 | 1:BI:534:VAL:HG22 | 2.18 | 0.44 |
| 2:BJ:114:ILE:HG23 | 2:BJ:115:GLU:H | 1.83 | 0.44 |
| 2:BJ:168:ILE:CG2 | 2:BJ:169:GLY:N | 2.81 | 0.44 |
| 2:BJ:338:PHE:CE2 | 2:BJ:342:SER:O | 2.69 | 0.44 |
| 2:BJ:511:GLU:N | 2:BJ:512:PRO:HD2 | 2.32 | 0.44 |
| 2:BJ:546:GLU:N | 2:BJ:546:GLU:OE1 | 2.49 | 0.44 |
| 2:BJ:549:PRO:HB2 | 2:BJ:550:GLU:OE1 | 2.17 | 0.44 |
| 2:C:160:VAL:O | 2:C:163:ILE:HB | 2.18 | 0.44 |
| 2:C:478:GLU:HG3 | 2:C:488:MET:SD | 2.58 | 0.44 |
| 3:CA:17:ARG:NH1 | 3:CA:334:PHE:O | 2.51 | 0.44 |
| 3:CB:135:ASP:H | 3:CB:187:VAL:HG12 | 1.82 | 0.44 |
| 3:CB:178:GLY:O | 3:CB:180:ILE:N | 2.51 | 0.44 |
| 4:CC:111:ASN:HB2 | 4:CC:116:ILE:HD12 | 1.98 | 0.44 |
| 4:CD:145:LYS:N | 4:CD:165:GLU:O | 2.49 | 0.44 |
| 4:CE:152:SER:O | 4:CE:158:SER:HA | 2.18 | 0.44 |
| 4:CE:192:PHE:CE1 | 4:CE:197:TYR:HB2 | 2.53 | 0.44 |
| 5:CF:150:GLN:HG3 | 5:CF:151:ILE:O | 2.18 | 0.44 |
| 5:CF:160:SER:HB3 | 5:CG:161:ASN:ND2 | 2.21 | 0.44 |
| 5:CH:320:LEU:HG | 5:CH:357:SER:HB3 | 2.00 | 0.44 |
| 6:CJ:195:LEU:HD13 | 6:CJ:215:PHE:CE1 | 2.52 | 0.44 |
| 3:D:66:LEU:HD11 | 2:GF:448:PHE:CE2 | 2.52 | 0.44 |
| 3:D:72:TRP:CE2 | 3:D:305:HIS:HA | 2.53 | 0.44 |
| 6:DA:91:SER:OG | 6:DA:177:THR:HB | 2.18 | 0.44 |
| 7:DB:301:ARG:O | 7:DD:295:ILE:HA | 2.17 | 0.44 |
| 7:DC:198:GLN:HA | 7:DC:201:GLN:CD | 2.38 | 0.44 |
| 8:DE:3:VAL:HG12 | 8:DF:58:ILE:HG23 | 1.98 | 0.44 |
| 8:DF:14:ASP:CG | 8:DF:17:ARG:HH22 | 2.18 | 0.44 |
| 1:EA:557:PRO:HB3 | 1:EA:589:TYR:CZ | 2.53 | 0.44 |
| 1:EB:374:ILE:HB | 1:EB:408:ILE:HG12 | 1.99 | 0.44 |
| 1:EB:533:ASP:OD1 | 1:EB:534:VAL:HG22 | 2.18 | 0.44 |
| 2:EC:494:GLU:HG3 | 2:EC:498:TRP:CG | 2.53 | 0.44 |
| 2:EC:515:ASN:OD1 | 2:EC:524:CYS:HB3 | 2.17 | 0.44 |
| 2:EC:912:ILE:HD11 | 3:ED:329:ASN:HD22 | 1.82 | 0.44 |
| 2:EC:84:THR:O | 2:EC:91:GLN:NE2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:60:TYR:N | 3:EE:9:ARG:HH11 | 2.16 | 0.44 |
| 3:ED:289:ASN:ND2 | 3:EE:233:GLN:HB2 | 2.33 | 0.44 |
| 4:EF:1:MET:HG2 | 4:EF:70:HIS:ND1 | 2.32 | 0.44 |
| 4:EG:67:TYR:CE1 | 4:EG:84:ARG:HD3 | 2.52 | 0.44 |
| 4:EH:192:PHE:CE1 | 4:EH:197:TYR:HB2 | 2.53 | 0.44 |
| 4:EH:67:TYR:CD1 | 4:EH:84:ARG:HB3 | 2.50 | 0.44 |
| 5:EJ:147:LYS:HG2 | 5:FA:154:ILE:O | 2.18 | 0.44 |
| 5:EJ:339:GLU:HG2 | 6:FD:173:THR:HB | 1.99 | 0.44 |
| 5:EI:386:PHE:CZ | 5:EJ:390:LEU:HD13 | 2.52 | 0.44 |
| 4:F:192:PHE:CE1 | 4:F:197:TYR:HB2 | 2.53 | 0.44 |
| 5:EI:279:SER:HB2 | 5:FA:326:MET:HB2 | 1.99 | 0.44 |
| 5:FA:469:PRO:HD3 | 5:FA:598:TRP:CE2 | 2.53 | 0.44 |
| 6:FC:130:ARG:O | 6:FC:134:GLN:HG3 | 2.18 | 0.44 |
| 7:FE:329:ASN:OD1 | 7:FE:330:ARG:N | 2.50 | 0.44 |
| 7:FE:435:GLY:HA2 | 7:FG:517:ILE:HD11 | 2.00 | 0.44 |
| 7:FF:173:ILE:HD12 | 7:FF:176:ILE:HG21 | 1.99 | 0.44 |
| 7:FF:32:VAL:HG22 | 7:FF:36:ILE:HG12 | 1.99 | 0.44 |
| 7:FG:88:PRO:HG2 | 7:FG:95:TYR:O | 2.16 | 0.44 |
| 9:FJ:10:ASP:OD1 | 9:FJ:11:ILE:HG22 | 2.18 | 0.44 |
| 4:G:192:PHE:CE1 | 4:G:197:TYR:HB2 | 2.53 | 0.44 |
| 11:GB:186:ARG:HG2 | 11:GB:187:ILE:H | 1.82 | 0.44 |
| 1:GD:69:GLN:CD | 1:GE:21:PHE:HZ | 2.21 | 0.44 |
| 1:GE:491:PHE:HE2 | 1:GE:619:GLN:HA | 1.82 | 0.44 |
| 1:GE:610:ASN:ND2 | 2:GF:804:ASN:HA | 2.33 | 0.44 |
| 3:GG:128:TRP:HB2 | 3:GG:194:ILE:HB | 1.99 | 0.44 |
| 4:GI:152:SER:O | 4:GI:158:SER:HA | 2.18 | 0.44 |
| 4:GJ:1:MET:HG2 | 4:GJ:70:HIS:ND1 | 2.32 | 0.44 |
| 4:HA:192:PHE:CE1 | 4:HA:197:TYR:HB2 | 2.53 | 0.44 |
| 5:HB:104:VAL:HG13 | 5:HB:105:ASN:H | 1.83 | 0.44 |
| 5:HB:248:MET:HB2 | 5:HB:254:TRP:CD1 | 2.52 | 0.44 |
| 5:HB:262:GLN:HA | 5:HB:381:ILE:O | 2.17 | 0.44 |
| 5:HB:288:MET:HG2 | 5:HB:289:LYS:O | 2.18 | 0.44 |
| 5:HB:293:PHE:HA | 5:HB:295:ALA:H | 1.82 | 0.44 |
| 5:HC:126:ILE:HD12 | 5:HC:133:LEU:HD11 | 1.98 | 0.44 |
| 5:HC:206:PHE:HB3 | 5:HC:223:VAL:HG13 | 1.99 | 0.44 |
| 5:HD:158:ASP:OD1 | 5:HD:159:ILE:N | 2.47 | 0.44 |
| 6:HF:107:VAL:HG22 | 6:HF:174:TYR:HD2 | 1.82 | 0.44 |
| 6:HG:73:ASN:ND2 | 6:HG:215:PHE:HE2 | 2.16 | 0.44 |
| 7:HH:160:MET:HG3 | 7:HH:164:LYS:HZ1 | 1.82 | 0.44 |
| 7:HI:32:VAL:HG22 | 7:HI:36:ILE:HG12 | 1.99 | 0.44 |
| 7:HJ:133:VAL:HA | 7:HJ:141:VAL:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:103:ASN:O | 5:I:104:VAL:C | 2.56 | 0.44 |
| 5:I:192:ARG:HG3 | 5:I:245:GLU:HB2 | 1.99 | 0.44 |
| 5:I:302:GLU:HG3 | 5:I:303:PRO:HD2 | 2.00 | 0.44 |
| 5:J:177:PHE:HD2 | 5:J:230:ILE:HD11 | 1.83 | 0.44 |
| 5:J:206:PHE:HB3 | 5:J:223:VAL:HG13 | 1.99 | 0.44 |
| 6:L:144:ASN:HB3 | 6:L:159:THR:HG22 | 1.99 | 0.44 |
| 6:M:91:SER:OG | 6:M:177:THR:HB | 2.18 | 0.44 |
| 6:L:13:ARG:NH1 | 6:N:47:PHE:CZ | 2.84 | 0.44 |
| 7:O:167:GLN:O | 7:O:171:LYS:HG2 | 2.18 | 0.44 |
| 7:O:371:ASP:OD1 | 7:O:526:LYS:NZ | 2.47 | 0.44 |
| 7:O:63:GLU:O | 7:O:67:ILE:HG12 | 2.18 | 0.44 |
| 7:P:99:ARG:HG2 | 7:P:100:TYR:O | 2.17 | 0.44 |
| 7:O:17:LYS:H | 7:Q:11:ASN:HB2 | 1.83 | 0.44 |
| 7:Q:272:GLN:NE2 | 7:Q:277:ALA:HA | 2.33 | 0.44 |
| 7:Q:67:ILE:HA | 7:Q:84:ARG:NH2 | 2.31 | 0.44 |
| 1:A:53:LEU:HB2 | 9:T:23:VAL:HG23 | 1.99 | 0.44 |
| 9:T:33:LYS:HG2 | 9:T:122:ILE:HG21 | 1.99 | 0.44 |
| 1:Y:256:TYR:CD1 | 1:Y:256:TYR:N | 2.83 | 0.44 |
| 13:YA:236[E]:ILE:HG23 | 13:YA:240[E]:GLU:HB2 | 1.99 | 0.44 |
| 13:YA:314[C]:SER:OG | 13:YA:316[C]:TRP:HB3 | 2.18 | 0.44 |
| 13:YA:330[C]:ILE:HD12 | 13:YA:336[C]:LEU:HD12 | 2.00 | 0.44 |
| 13:YA:450[F]:VAL:O | 13:YC:459[F]:GLY:N | 2.50 | 0.44 |
| 13:YB:109[A]:ASN:OD1 | 13:YB:110[A]:ARG:N | 2.51 | 0.44 |
| 13:YB:112[B]:GLU:C | 13:YB:115[B]:SER:HB3 | 2.38 | 0.44 |
| 13:YB:263[B]:GLY:N | 13:YB:264[B]:PRO:HD2 | 2.33 | 0.44 |
| 13:YB:50[C]:GLU:N | 13:YB:50[C]:GLU:CD | 2.71 | 0.44 |
| 13:YB:534[A]:LEU:HD11 | 13:YB:536[A]:TRP:NE1 | 2.32 | 0.44 |
| 13:YB:534[D]:LEU:HD11 | 13:YB:536[D]:TRP:NE1 | 2.32 | 0.44 |
| 13:YB:61[F]:ILE:HG21 | 13:YC:59[F]:GLN:HA | 1.99 | 0.44 |
| 13:YB:92[D]:THR:HB | 14:YE:282[D]:ALA:CB | 2.48 | 0.44 |
| 13:YA:473[D]:GLN:OE1 | 13:YC:158[D]:PRO:HB2 | 2.18 | 0.44 |
| 13:YC:263[F]:GLY:N | 13:YC:264[F]:PRO:HD2 | 2.33 | 0.44 |
| 13:YA:438[D]:LEU:CD2 | 13:YC:442[D]:THR:HG21 | 2.48 | 0.44 |
| 13:YA:551[A]:THR:HA | 13:YC:558[A]:SER:O | 2.18 | 0.44 |
| 13:YC:61[C]:ILE:HG13 | 13:YC:62[C]:THR:N | 2.27 | 0.44 |
| 13:YC:76[C]:PRO:HB2 | 13:YC:97[C]:LEU:C | 2.38 | 0.44 |
| 14:YD:127[B]:ASP:CG | 14:YD:130[B]:GLU:H | 2.20 | 0.44 |
| 14:YD:140[A]:TYR:HE2 | 14:YD:148[A]:PRO:HD3 | 1.83 | 0.44 |
| 14:YD:279[F]:ARG:HA | 14:YD:279[F]:ARG:HD3 | 1.43 | 0.44 |
| 14:YE:233[D]:ASP:N | 14:YE:233[D]:ASP:OD1 | 2.51 | 0.44 |
| 14:YE:88[F]:TYR:HD1 | 14:YE:110[F]:GLY:C | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:236[F]:TRP:N | 14:YE:95[F]:VAL:O | 2.51 | 0.44 |
| 14:YF:233[B]:ASP:N | 14:YF:233[B]:ASP:OD1 | 2.51 | 0.44 |
| 14:YF:308[A]:ALA:O | 14:YF:357[A]:MET:N | 2.51 | 0.44 |
| 14:YF:73[C]:SER:HA | 14:YF:85[C]:THR:HA | 2.00 | 0.44 |
| 2:Z:52:ASN:O | 2:Z:54:TYR:N | 2.51 | 0.44 |
| 2:Z:865:LYS:HE3 | 2:Z:893:ILE:HD12 | 1.99 | 0.44 |
| 2:Z:982:LEU:HD12 | 2:Z:982:LEU:O | 2.17 | 0.44 |
| 1:A:113:THR:O | 1:A:298:ILE:HG13 | 2.18 | 0.44 |
| 4:AA:152:SER:O | 4:AA:158:SER:HA | 2.18 | 0.44 |
| 4:AA:192:PHE:CE1 | 4:AA:197:TYR:HB2 | 2.53 | 0.44 |
| 4:AB:1:MET:HG2 | 4:AB:70:HIS:ND1 | 2.32 | 0.44 |
| 5:AC:129:ARG:HG3 | 5:AC:130:PHE:N | 2.30 | 0.44 |
| 5:AC:153:LYS:HE3 | 5:AC:155:THR:OG1 | 2.17 | 0.44 |
| 5:AC:213:GLY:CA | 5:AC:221:GLU:HB2 | 2.47 | 0.44 |
| 5:AD:115:ASP:OD2 | 5:AD:137:TYR:HE1 | 2.01 | 0.44 |
| 5:AC:569:TYR:HB2 | 5:AD:550:VAL:HB | 2.00 | 0.44 |
| 5:AD:71:ASN:HB2 | 5:AD:99:PHE:HZ | 1.82 | 0.44 |
| 5:AD:49:TRP:CZ3 | 5:AD:96:ARG:HD2 | 2.52 | 0.44 |
| 5:AE:135:LEU:HA | 5:AE:144:GLU:O | 2.18 | 0.44 |
| 5:AE:352:SER:HB2 | 5:AE:354:THR:O | 2.18 | 0.44 |
| 6:AG:108:LEU:HD23 | 6:AG:113:PRO:HA | 2.00 | 0.44 |
| 6:AH:144:ASN:HB3 | 6:AH:159:THR:HG22 | 1.99 | 0.44 |
| 7:AI:111:ASN:CG | 7:AI:114:SER:HB3 | 2.38 | 0.44 |
| 7:AI:125:LEU:O | 7:AI:129:PHE:N | 2.45 | 0.44 |
| 7:AI:94:VAL:HG12 | 7:AI:95:TYR:O | 2.18 | 0.44 |
| 7:AJ:129:PHE:CE2 | 7:AJ:141:VAL:HG11 | 2.52 | 0.44 |
| 1:B:205:GLU:C | 1:B:206:TRP:HD1 | 2.21 | 0.44 |
| 7:BA:168:LEU:HA | 7:BA:168:LEU:HD23 | 1.79 | 0.44 |
| 7:BA:240:ASN:HB3 | 7:BA:243:VAL:HG22 | 2.00 | 0.44 |
| 7:BA:20:PRO:CB | 7:BA:29:ILE:HG13 | 2.48 | 0.44 |
| 7:AI:448:ALA:HA | 7:BA:483:PHE:HA | 2.00 | 0.44 |
| 7:AI:97:LEU:HD23 | 7:BA:97:LEU:CD2 | 2.48 | 0.44 |
| 11:BF:74:LEU:HA | 11:BF:74:LEU:HD12 | 1.78 | 0.44 |
| 11:BF:36:PHE:HZ | 11:BF:76:CYS:SG | 2.40 | 0.44 |
| 1:BH:345:TYR:OH | 1:BH:400:ASN:ND2 | 2.51 | 0.44 |
| 1:BH:347:THR:O | 1:BH:351:GLU:N | 2.43 | 0.44 |
| 1:BI:348:PHE:HZ | 1:BI:399:TYR:CD2 | 2.35 | 0.44 |
| 1:BI:486:ARG:NH2 | 1:BI:500:LYS:O | 2.51 | 0.44 |
| 2:BJ:213:ASN:HB2 | 2:BJ:289:PHE:CZ | 2.53 | 0.44 |
| 2:BJ:400:ASP:O | 2:BJ:424:ARG:NH1 | 2.50 | 0.44 |
| 1:BH:79:PHE:CE1 | 2:BJ:702:GLU:HG2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:777:LEU:HD23 | 2:BJ:809:TRP:CD2 | 2.53 | 0.44 |
| 2:BJ:927:THR:HB | 2:BJ:987:ARG:HA | 2.00 | 0.44 |
| 2:C:168:ILE:CG2 | 2:C:169:GLY:N | 2.81 | 0.44 |
| 2:C:37:GLU:O | 2:C:80:ILE:HA | 2.17 | 0.44 |
| 2:C:865:LYS:HE3 | 2:C:893:ILE:HD12 | 1.99 | 0.44 |
| 3:CA:289:ASN:ND2 | 3:CB:233:GLN:HB2 | 2.33 | 0.44 |
| 4:CE:145:LYS:N | 4:CE:165:GLU:O | 2.49 | 0.44 |
| 5:CF:267:ASP:CG | 5:CF:285:LEU:HB2 | 2.38 | 0.44 |
| 5:CF:290:SER:HA | 5:CF:371:PHE:H | 1.82 | 0.44 |
| 5:CF:302:GLU:HG3 | 5:CF:303:PRO:HD2 | 2.00 | 0.44 |
| 5:CF:402:GLU:HG2 | 5:CH:396:LYS:HE3 | 1.99 | 0.44 |
| 5:CG:323:THR:HG22 | 5:CG:355:ASP:O | 2.18 | 0.44 |
| 5:CH:318:GLN:HB3 | 6:CJ:4:LEU:CG | 2.47 | 0.44 |
| 5:CG:551:ILE:HD13 | 5:CH:565:ILE:CD1 | 2.46 | 0.44 |
| 6:CI:130:ARG:O | 6:CI:134:GLN:HG3 | 2.18 | 0.44 |
| 3:D:115:ASN:HD21 | 3:D:123:GLU:HB3 | 1.83 | 0.44 |
| 3:D:92:ARG:HD3 | 3:D:205:ASN:O | 2.18 | 0.44 |
| 3:D:274:ILE:HD12 | 3:D:311:TYR:HB3 | 1.99 | 0.44 |
| 7:DB:476:ASP:OD1 | 7:DB:479:ASN:ND2 | 2.50 | 0.44 |
| 7:DC:117:THR:HG22 | 7:DC:120:LYS:NZ | 2.32 | 0.44 |
| 7:DB:44:VAL:HB | 7:DC:24:ASN:ND2 | 2.32 | 0.44 |
| 7:DD:23:THR:OG1 | 7:DD:25:PHE:O | 2.26 | 0.44 |
| 7:DD:272:GLN:NE2 | 7:DD:277:ALA:HA | 2.33 | 0.44 |
| 7:DB:469:VAL:HB | 7:DD:477:TRP:CZ3 | 2.53 | 0.44 |
| 9:DG:10:ASP:OD1 | 9:DG:11:ILE:HG22 | 2.18 | 0.44 |
| 10:DH:203:ARG:NH1 | 10:DH:311:PHE:HE1 | 2.16 | 0.44 |
| 11:DI:44:ARG:HG2 | 11:DI:45:LEU:N | 2.33 | 0.44 |
| 3:E:232:GLN:O | 3:E:233:GLN:HB2 | 2.18 | 0.44 |
| 1:EB:358:GLN:HB2 | 1:EB:379:LYS:HD3 | 2.00 | 0.44 |
| 1:EB:610:ASN:ND2 | 2:EC:804:ASN:HA | 2.33 | 0.44 |
| 3:ED:150:LYS:HA | 3:ED:160:TRP:CZ3 | 2.53 | 0.44 |
| 3:ED:150:LYS:HE2 | 3:ED:160:TRP:CD1 | 2.53 | 0.44 |
| 3:ED:130:VAL:HG21 | 3:ED:192:PHE:CZ | 2.53 | 0.44 |
| 3:EE:135:ASP:H | 3:EE:187:VAL:HG12 | 1.82 | 0.44 |
| 4:EF:164:ILE:O | 4:EH:171:LYS:N | 2.44 | 0.44 |
| 4:EF:54:THR:HA | 4:EG:7:LYS:O | 2.18 | 0.44 |
| 5:EI:150:GLN:HG3 | 5:EI:151:ILE:O | 2.18 | 0.44 |
| 5:EI:193:VAL:O | 5:EI:199:GLU:N | 2.46 | 0.44 |
| 5:EI:262:GLN:HA | 5:EI:381:ILE:O | 2.18 | 0.44 |
| 5:EI:535:THR:OG1 | 5:FA:576:THR:HB | 2.18 | 0.44 |
| 5:EJ:115:ASP:OD2 | 5:EJ:137:TYR:HE1 | 2.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:68:GLN:HB3 | 4:F:70:HIS:NE2 | 2.32 | 0.44 |
| 5:EJ:542:LEU:HD21 | 5:FA:569:TYR:OH | 2.18 | 0.44 |
| 5:FA:340:VAL:HG22 | 6:FB:173:THR:HA | 1.98 | 0.44 |
| 6:FB:91:SER:OG | 6:FB:177:THR:HB | 2.18 | 0.44 |
| 5:EI:318:GLN:HB3 | 6:FD:4:LEU:HD12 | 1.99 | 0.44 |
| 7:FF:375:TYR:CZ | 7:FF:392:LEU:HD23 | 2.53 | 0.44 |
| 7:FF:516:ASN:ND2 | 7:FG:401:ARG:HD2 | 2.33 | 0.44 |
| 7:FG:21:THR:OG1 | 7:FG:22:ASP:N | 2.51 | 0.44 |
| 8:BB:2:PHE:CD2 | 8:FI:98:GLU:HA | 2.53 | 0.44 |
| 9:FJ:114:ASP:O | 11:IE:47:THR:OG1 | 2.36 | 0.44 |
| 9:FJ:75:ARG:HG3 | 10:GA:123:PRO:HG3 | 1.99 | 0.44 |
| 1:GD:53:LEU:HB2 | 9:IC:23:VAL:HG23 | 1.99 | 0.44 |
| 1:GE:332:LYS:O | 1:GE:335:THR:HG22 | 2.18 | 0.44 |
| 2:GF:114:ILE:HG23 | 2:GF:115:GLU:N | 2.33 | 0.44 |
| 2:GF:450:PHE:HE2 | 2:GF:473:TYR:HH | 1.65 | 0.44 |
| 2:GF:494:GLU:HG3 | 2:GF:498:TRP:CG | 2.53 | 0.44 |
| 2:GF:934:ALA:H | 2:GF:997:SER:CB | 2.31 | 0.44 |
| 3:GG:130:VAL:HG21 | 3:GG:192:PHE:CZ | 2.53 | 0.44 |
| 3:GH:79:VAL:HG12 | 3:GH:80:LYS:O | 2.18 | 0.44 |
| 5:HB:214:SER:HB2 | 5:HB:215:PRO:HD2 | 1.98 | 0.44 |
| 5:HB:384:THR:O | 5:HB:385:TRP:HD1 | 2.01 | 0.44 |
| 5:HB:402:GLU:HG3 | 5:HB:406:LEU:CD1 | 2.47 | 0.44 |
| 5:HC:11:VAL:HG13 | 5:HD:20:ARG:HG2 | 1.99 | 0.44 |
| 5:HC:340:VAL:HG22 | 6:HG:172:SER:O | 2.18 | 0.44 |
| 5:HC:359:GLU:O | 5:HC:370:HIS:N | 2.45 | 0.44 |
| 5:HC:305:ASN:HB3 | 5:HD:255:ARG:NH1 | 2.33 | 0.44 |
| 5:HB:98:VAL:HG22 | 5:HD:90:ASN:HA | 1.99 | 0.44 |
| 6:HE:91:SER:OG | 6:HE:177:THR:HB | 2.18 | 0.44 |
| 6:HF:130:ARG:O | 6:HF:134:GLN:HG3 | 2.18 | 0.44 |
| 6:HG:130:ARG:O | 6:HG:134:GLN:HG3 | 2.18 | 0.44 |
| 6:HG:88:TRP:O | 6:HG:155:LYS:HA | 2.18 | 0.44 |
| 7:HJ:21:THR:OG1 | 7:HJ:22:ASP:N | 2.51 | 0.44 |
| 7:HJ:359:TRP:CZ2 | 7:HJ:524:LYS:HD3 | 2.52 | 0.44 |
| 7:HH:39:ILE:HD13 | 7:HJ:39:ILE:HD13 | 1.99 | 0.44 |
| 5:I:214:SER:HB2 | 5:I:215:PRO:HD2 | 1.98 | 0.44 |
| 5:I:290:SER:CA | 5:I:371:PHE:H | 2.30 | 0.44 |
| 8:R:94:GLY:O | 8:IA:64:ARG:HD2 | 2.18 | 0.44 |
| 9:IC:56:ASP:OD2 | 10:ID:32:LYS:HE2 | 2.17 | 0.44 |
| 12:IF:99:SER:HB3 | 12:IF:102:GLY:O | 2.17 | 0.44 |
| 5:J:129:ARG:HG3 | 5:J:130:PHE:N | 2.33 | 0.44 |
| 5:I:248:MET:HE3 | 5:J:254:TRP:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:34:TYR:OH | 5:J:42:VAL:N | 2.50 | 0.44 |
| 5:J:71:ASN:HB2 | 5:J:99:PHE:HZ | 1.82 | 0.44 |
| 5:K:137:TYR:HD1 | 5:K:143:TRP:HE1 | 1.61 | 0.44 |
| 5:K:135:LEU:HA | 5:K:144:GLU:O | 2.18 | 0.44 |
| 5:K:318:GLN:HB3 | 6:M:4:LEU:CG | 2.48 | 0.44 |
| 5:K:320:LEU:HG | 5:K:357:SER:HB3 | 2.00 | 0.44 |
| 5:I:46:ALA:N | 5:K:65:GLY:O | 2.35 | 0.44 |
| 6:M:88:TRP:O | 6:M:155:LYS:HA | 2.18 | 0.44 |
| 6:N:144:ASN:HB3 | 6:N:159:THR:HG22 | 1.99 | 0.44 |
| 6:N:88:TRP:O | 6:N:155:LYS:HA | 2.18 | 0.44 |
| 7:P:198:GLN:HA | 7:P:201:GLN:CD | 2.38 | 0.44 |
| 7:P:368:SER:HA | 7:P:389:ASN:ND2 | 2.32 | 0.44 |
| 7:P:375:TYR:CZ | 7:P:392:LEU:HD23 | 2.53 | 0.44 |
| 7:Q:407:SER:HA | 7:Q:410:THR:OG1 | 2.17 | 0.44 |
| 7:Q:445:HIS:CD2 | 7:Q:447:HIS:CE1 | 3.06 | 0.44 |
| 8:R:32:PHE:O | 8:R:35:GLN:N | 2.50 | 0.44 |
| 8:R:5:ASP:HA | 8:R:8:ARG:HB3 | 2.00 | 0.44 |
| 9:T:96:ILE:O | 9:T:105:ILE:HG22 | 2.17 | 0.44 |
| 10:U:37:GLN:HB3 | 10:U:128:LEU:HB3 | 1.99 | 0.44 |
| 11:V:2:LEU:HD23 | 11:V:32:TYR:CD1 | 2.53 | 0.44 |
| 1:Y:634:THR:HB | 1:Y:638:SER:O | 2.17 | 0.44 |
| 13:YA:110[E]:ARG:HD2 | 13:YA:118[E]:THR:O | 2.17 | 0.44 |
| 13:YA:219[D]:LYS:HB2 | 13:YA:219[D]:LYS:HE3 | 1.81 | 0.44 |
| 13:YA:478[B]:ASN:N | 13:YC:485[B]:ASP:O | 2.49 | 0.44 |
| 13:YA:552[E]:GLU:CG | 13:YA:554[E]:MET:HE1 | 2.48 | 0.44 |
| 13:YA:558[D]:SER:N | 13:YB:550[D]:TRP:O | 2.50 | 0.44 |
| 13:YA:565[B]:TYR:CZ | 13:YB:557[B]:MET:HG2 | 2.53 | 0.44 |
| 13:YB:109[E]:ASN:OD1 | 13:YB:110[E]:ARG:N | 2.51 | 0.44 |
| 13:YB:147[E]:ILE:HD11 | 13:YB:188[E]:LEU:HG | 2.00 | 0.44 |
| 13:YB:24[A]:LEU:HD21 | 13:YC:102[A]:GLY:HA2 | 2.00 | 0.44 |
| 13:YB:261[D]:LYS:HE2 | 13:YB:293[D]:ASN:HB3 | 1.99 | 0.44 |
| 13:YB:320[D]:THR:HG22 | 13:YB:323[D]:ARG:HB3 | 2.00 | 0.44 |
| 13:YA:376[C]:PHE:CD2 | 13:YB:447[C]:ASN:OD1 | 2.71 | 0.44 |
| 13:YA:376[E]:PHE:CD2 | 13:YB:447[E]:ASN:OD1 | 2.71 | 0.44 |
| 13:YB:458[C]:VAL:HG21 | 13:YC:454[C]:LYS:HD2 | 2.00 | 0.44 |
| 13:YB:521[E]:LEU:HD12 | 13:YB:522[E]:VAL:N | 2.32 | 0.44 |
| 13:YB:552[B]:GLU:CG | 13:YB:554[B]:MET:HE1 | 2.48 | 0.44 |
| 13:YC:109[F]:ASN:OD1 | 13:YC:110[F]:ARG:N | 2.51 | 0.44 |
| 13:YC:112[E]:GLU:C | 13:YC:115[E]:SER:HB3 | 2.38 | 0.44 |
| 13:YB:71[C]:GLY:HA2 | 13:YC:393[C]:MET:HA | 2.00 | 0.44 |
| 13:YC:521[F]:LEU:HD12 | 13:YC:522[F]:VAL:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:544[C]:TRP:HB2 | 13:YC:552[C]:GLU:HB2 | 2.00 | 0.44 |
| 13:YA:544[D]:TRP:HB2 | 13:YC:552[D]:GLU:HB2 | 2.00 | 0.44 |
| 13:YA:551[C]:THR:HA | 13:YC:558[C]:SER:O | 2.18 | 0.44 |
| 14:YD:140[D]:TYR:HE2 | 14:YD:148[D]:PRO:HD3 | 1.82 | 0.44 |
| 14:YD:234[E]:PHE:HD1 | 14:YE:97[E]:VAL:HG12 | 1.82 | 0.44 |
| 14:YD:277[F]:VAL:HG11 | 14:YD:294[F]:GLU:HG2 | 1.99 | 0.44 |
| 14:YE:109[B]:LEU:HA | 14:YE:109[B]:LEU:HD12 | 1.65 | 0.44 |
| 14:YE:140[A]:TYR:HE2 | 14:YE:148[A]:PRO:HD3 | 1.83 | 0.44 |
| 13:YB:26[A]:ARG:HD3 | 14:YE:259[A]:LEU:HD21 | 2.00 | 0.44 |
| 14:YE:308[B]:ALA:O | 14:YE:357[B]:MET:N | 2.51 | 0.44 |
| 14:YE:308[F]:ALA:O | 14:YE:357[F]:MET:N | 2.51 | 0.44 |
| 14:YE:38[B]:LEU:HD12 | 14:YE:38[B]:LEU:HA | 1.63 | 0.44 |
| 14:YF:127[B]:ASP:CG | 14:YF:130[B]:GLU:H | 2.20 | 0.44 |
| 14:YF:140[A]:TYR:HE2 | 14:YF:148[A]:PRO:HD3 | 1.83 | 0.44 |
| 14:YD:95[E]:VAL:O | 14:YF:236[E]:TRP:N | 2.51 | 0.44 |
| 14:YF:308[F]:ALA:O | 14:YF:357[F]:MET:N | 2.51 | 0.44 |
| 14:YF:44[E]:LEU:HB2 | 14:YF:340[E]:ASP:O | 2.18 | 0.44 |
| 2:Z:145:ALA:O | 2:Z:586:LEU:HB3 | 2.18 | 0.44 |
| 2:Z:934:ALA:H | 2:Z:997:SER:CB | 2.31 | 0.44 |
| 1:A:432:SER:O | 1:A:435:TRP:HB3 | 2.18 | 0.44 |
| 4:AB:152:SER:O | 4:AB:158:SER:HA | 2.18 | 0.44 |
| 5:AC:549:SER:N | 5:AE:569:TYR:O | 2.51 | 0.44 |
| 5:AD:135:LEU:HA | 5:AD:144:GLU:O | 2.18 | 0.44 |
| 5:AD:36:GLU:HA | 5:AD:50:LYS:HZ2 | 1.83 | 0.44 |
| 6:AF:88:TRP:O | 6:AF:155:LYS:HA | 2.18 | 0.44 |
| 7:AI:301:ARG:O | 7:BA:295:ILE:HA | 2.17 | 0.44 |
| 7:AI:476:ASP:OD1 | 7:AI:479:ASN:ND2 | 2.50 | 0.44 |
| 7:AJ:126:ASN:O | 7:AJ:129:PHE:HB3 | 2.18 | 0.44 |
| 7:AJ:445:HIS:CE1 | 7:BA:447:HIS:CE1 | 3.06 | 0.44 |
| 7:AI:475:LEU:HA | 7:AJ:470:GLY:O | 2.18 | 0.44 |
| 7:AJ:77:THR:CG2 | 7:AJ:80:THR:H | 2.31 | 0.44 |
| 1:B:486:ARG:NH2 | 1:B:500:LYS:O | 2.51 | 0.44 |
| 1:B:634:THR:HB | 1:B:638:SER:O | 2.17 | 0.44 |
| 7:AI:473:LYS:CD | 7:BA:473:LYS:HB3 | 2.43 | 0.44 |
| 11:BF:66:ASN:OD1 | 11:BF:68:GLN:N | 2.42 | 0.44 |
| 1:BH:278:ALA:HB2 | 1:BH:317:GLY:N | 2.33 | 0.44 |
| 1:BI:491:PHE:HE2 | 1:BI:619:GLN:HA | 1.82 | 0.44 |
| 2:BJ:193:MET:O | 2:BJ:200:TYR:N | 2.36 | 0.44 |
| 2:BJ:612:TRP:CD1 | 2:BJ:618:PHE:HB3 | 2.53 | 0.44 |
| 1:BH:341:THR:HG23 | 2:BJ:880:ILE:O | 2.18 | 0.44 |
| 2:BJ:84:THR:O | 2:BJ:91:GLN:NE2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:110:PHE:HB3 | 2:C:621:ALA:HA | 1.99 | 0.44 |
| 2:C:511:GLU:N | 2:C:512:PRO:HD2 | 2.33 | 0.44 |
| 2:C:52:ASN:O | 2:C:54:TYR:N | 2.51 | 0.44 |
| 2:C:934:ALA:H | 2:C:997:SER:CB | 2.31 | 0.44 |
| 3:CB:294:LYS:HB2 | 3:CB:297:TYR:CZ | 2.53 | 0.44 |
| 4:CC:145:LYS:N | 4:CC:165:GLU:O | 2.49 | 0.44 |
| 5:CG:304:ILE:HD11 | 5:CG:309:LEU:HA | 2.00 | 0.44 |
| 5:CG:34:TYR:OH | 5:CG:42:VAL:N | 2.50 | 0.44 |
| 5:CH:309:LEU:HD23 | 5:CH:310:GLU:N | 2.33 | 0.44 |
| 5:CF:408:VAL:HG23 | 5:CH:409:SER:O | 2.18 | 0.44 |
| 6:CI:108:LEU:HD23 | 6:CI:113:PRO:HA | 2.00 | 0.44 |
| 5:CH:340:VAL:HG22 | 6:CI:173:THR:HA | 1.99 | 0.44 |
| 6:CJ:88:TRP:O | 6:CJ:155:LYS:HA | 2.18 | 0.44 |
| 6:DA:108:LEU:HD23 | 6:DA:113:PRO:HA | 2.00 | 0.44 |
| 6:CI:10:VAL:HG11 | 6:DA:10:VAL:HG21 | 2.00 | 0.44 |
| 7:DB:288:ILE:O | 7:DC:288:ILE:N | 2.42 | 0.44 |
| 7:DB:78:PRO:HB2 | 7:DC:69:GLY:HA2 | 1.99 | 0.44 |
| 7:DB:190:VAL:HB | 7:DC:189:GLY:N | 2.33 | 0.44 |
| 7:DC:77:THR:CG2 | 7:DC:80:THR:H | 2.31 | 0.44 |
| 7:DD:2:SER:O | 7:DD:5:THR:HB | 2.18 | 0.44 |
| 1:BH:52:ARG:NH2 | 9:DG:25:ARG:HB3 | 2.33 | 0.44 |
| 12:DJ:220:SER:HA | 12:DJ:243:PHE:HD1 | 1.82 | 0.44 |
| 3:E:71:MET:SD | 3:E:312:MET:HG2 | 2.58 | 0.44 |
| 1:EA:10:LEU:O | 1:EA:11:THR:OG1 | 2.31 | 0.44 |
| 1:EA:113:THR:O | 1:EA:298:ILE:HG13 | 2.18 | 0.44 |
| 1:EA:365:ASP:OD2 | 1:EA:367:THR:HB | 2.18 | 0.44 |
| 2:EC:151:PHE:HB3 | 2:EC:166:PHE:HZ | 1.83 | 0.44 |
| 2:EC:478:GLU:HG3 | 2:EC:488:MET:SD | 2.58 | 0.44 |
| 3:ED:128:TRP:HB2 | 3:ED:194:ILE:HB | 1.99 | 0.44 |
| 3:ED:92:ARG:HD3 | 3:ED:205:ASN:O | 2.18 | 0.44 |
| 3:EE:140:GLY:HA2 | 3:EE:163:SER:N | 2.33 | 0.44 |
| 4:EF:83:THR:HA | 4:EH:63:ALA:HB3 | 1.99 | 0.44 |
| 5:EI:20:ARG:NH1 | 5:EI:24:ILE:HD12 | 2.32 | 0.44 |
| 5:EI:213:GLY:CA | 5:EI:221:GLU:HB2 | 2.47 | 0.44 |
| 5:EJ:202:TYR:OH | 5:EJ:223:VAL:O | 2.19 | 0.44 |
| 5:FA:470:VAL:O | 5:FA:474:GLY:N | 2.50 | 0.44 |
| 6:FC:88:TRP:O | 6:FC:155:LYS:HA | 2.18 | 0.44 |
| 6:FD:172:SER:HA | 6:FD:176:ILE:O | 2.17 | 0.44 |
| 7:FE:509:GLY:HA3 | 7:FF:441:GLN:HE21 | 1.83 | 0.44 |
| 7:FE:509:GLY:O | 7:FF:443:SER:HA | 2.18 | 0.44 |
| 7:FE:95:TYR:HD1 | 7:FG:99:ARG:N | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FF:478:ASP:CG | 7:FG:454:HIS:HE2 | 2.21 | 0.44 |
| 9:FJ:96:ILE:O | 9:FJ:105:ILE:HG22 | 2.17 | 0.44 |
| 10:GA:286:VAL:HG22 | 10:GA:287:VAL:N | 2.32 | 0.44 |
| 11:GB:175:SER:HA | 14:YD:217[E]:SER:HB2 | 1.99 | 0.44 |
| 11:GB:186:ARG:HG3 | 11:GB:187:ILE:N | 2.33 | 0.44 |
| 11:GB:31:ASN:O | 11:GB:32:TYR:HB2 | 2.18 | 0.44 |
| 1:GD:561:GLY:H | 1:GD:588:LYS:NZ | 2.16 | 0.44 |
| 2:GF:186:ASP:HB3 | 2:GF:189:ARG:HE | 1.83 | 0.44 |
| 2:GF:52:ASN:O | 2:GF:54:TYR:N | 2.51 | 0.44 |
| 3:GG:92:ARG:HD3 | 3:GG:205:ASN:O | 2.18 | 0.44 |
| 3:GH:135:ASP:H | 3:GH:187:VAL:HG12 | 1.82 | 0.44 |
| 4:HA:1:MET:HG2 | 4:HA:70:HIS:ND1 | 2.32 | 0.44 |
| 5:HB:184:THR:H | 5:HB:307:ASN:ND2 | 2.13 | 0.44 |
| 5:HB:285:LEU:HD11 | 5:HB:375:PHE:CB | 2.41 | 0.44 |
| 5:HB:290:SER:HA | 5:HB:371:PHE:H | 1.82 | 0.44 |
| 5:HB:89:TYR:CE1 | 5:HB:137:TYR:CZ | 3.06 | 0.44 |
| 5:HC:389:ASP:N | 5:HC:389:ASP:OD1 | 2.51 | 0.44 |
| 5:HD:309:LEU:HD23 | 5:HD:310:GLU:N | 2.33 | 0.44 |
| 5:HB:407:TYR:CD1 | 5:HD:407:TYR:HB2 | 2.53 | 0.44 |
| 6:HF:195:LEU:HD13 | 6:HF:215:PHE:CE1 | 2.52 | 0.44 |
| 6:HG:144:ASN:HB3 | 6:HG:159:THR:HG22 | 1.99 | 0.44 |
| 7:HI:375:TYR:CZ | 7:HI:392:LEU:HD23 | 2.53 | 0.44 |
| 7:HI:445:HIS:CE1 | 7:HJ:447:HIS:CE1 | 3.06 | 0.44 |
| 7:HJ:240:ASN:HB3 | 7:HJ:243:VAL:HG22 | 2.00 | 0.44 |
| 7:HJ:407:SER:HA | 7:HJ:410:THR:OG1 | 2.17 | 0.44 |
| 7:HH:473:LYS:CD | 7:HJ:473:LYS:HB3 | 2.43 | 0.44 |
| 7:HH:463:THR:HG23 | 7:HJ:483:PHE:HE1 | 1.82 | 0.44 |
| 7:HJ:2:SER:O | 7:HJ:5:THR:HB | 2.18 | 0.44 |
| 5:I:318:GLN:NE2 | 6:N:7:LYS:HB3 | 2.32 | 0.44 |
| 5:I:323:THR:HG21 | 5:I:354:THR:HG23 | 1.99 | 0.44 |
| 8:IA:22:GLN:OE1 | 8:IA:116:TYR:OH | 2.25 | 0.44 |
| 8:IA:98:GLU:N | 8:IA:98:GLU:OE1 | 2.48 | 0.44 |
| 5:I:569:TYR:HB2 | 5:J:550:VAL:HB | 2.00 | 0.44 |
| 5:K:309:LEU:HD23 | 5:K:310:GLU:N | 2.33 | 0.44 |
| 7:O:447:HIS:CE1 | 7:Q:445:HIS:CE1 | 3.05 | 0.44 |
| 7:Q:133:VAL:HA | 7:Q:141:VAL:O | 2.18 | 0.44 |
| 7:Q:20:PRO:CB | 7:Q:29:ILE:HG13 | 2.48 | 0.44 |
| 7:O:504:ARG:NH2 | 7:Q:424:ARG:O | 2.46 | 0.44 |
| 7:Q:2:SER:O | 7:Q:5:THR:HB | 2.18 | 0.44 |
| 1:X:446:ARG:NE | 1:X:450:GLU:OE2 | 2.51 | 0.44 |
| 1:Y:276:ASN:HB2 | 1:Y:279:ASP:OD2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:485:VAL:HG11 | 1:Y:650:TYR:CE1 | 2.53 | 0.44 |
| 1:Y:486:ARG:NH2 | 1:Y:500:LYS:O | 2.51 | 0.44 |
| 1:Y:508:ARG:HE | 1:Y:544:ASP:HB2 | 1.83 | 0.44 |
| 1:Y:56:LEU:HA | 2:Z:653:MET:HE1 | 2.00 | 0.44 |
| 13:YA:109[F]:ASN:OD1 | 13:YA:110[F]:ARG:N | 2.51 | 0.44 |
| 13:YA:236[C]:ILE:HG23 | 13:YA:240[C]:GLU:HB2 | 1.99 | 0.44 |
| 13:YA:257[D]:LYS:HE2 | 13:YA:266[D]:TRP:CH2 | 2.53 | 0.44 |
| 13:YA:314[D]:SER:OG | 13:YA:316[D]:TRP:HB3 | 2.17 | 0.44 |
| 13:YA:389[F]:TYR:O | 13:YA:405[F]:ASP:HB2 | 2.18 | 0.44 |
| 13:YA:473[C]:GLN:OE1 | 13:YC:158[C]:PRO:HB2 | 2.18 | 0.44 |
| 13:YA:76[D]:PRO:HG3 | 13:YA:96[D]:VAL:CG1 | 2.48 | 0.44 |
| 13:YB:112[F]:GLU:C | 13:YB:115[F]:SER:HB3 | 2.39 | 0.44 |
| 13:YB:236[C]:ILE:HG23 | 13:YB:240[C]:GLU:HB2 | 1.99 | 0.44 |
| 13:YB:257[A]:LYS:HE2 | 13:YB:266[A]:TRP:CH2 | 2.53 | 0.44 |
| 13:YB:321[C]:LYS:HD3 | 13:YC:452[C]:GLY:CA | 2.47 | 0.44 |
| 13:YB:36[B]:PRO:HB2 | 13:YB:38[B]:GLN:OE1 | 2.18 | 0.44 |
| 13:YB:66[E]:MET:HE2 | 13:YC:122[E]:PRO:HB3 | 2.00 | 0.44 |
| 13:YB:76[C]:PRO:HB2 | 13:YB:97[C]:LEU:C | 2.37 | 0.44 |
| 13:YB:76[A]:PRO:HG3 | 13:YB:96[A]:VAL:CG1 | 2.48 | 0.44 |
| 13:YC:109[C]:ASN:OD1 | 13:YC:110[C]:ARG:N | 2.51 | 0.44 |
| 13:YC:236[C]:ILE:HG23 | 13:YC:240[C]:GLU:HB2 | 1.99 | 0.44 |
| 13:YA:516[E]:GLY:O | 13:YC:522[E]:VAL:HG23 | 2.18 | 0.44 |
| 13:YC:521[C]:LEU:HD12 | 13:YC:522[C]:VAL:N | 2.32 | 0.44 |
| 13:YA:534[C]:LEU:CB | 13:YC:538[C]:VAL:HG11 | 2.47 | 0.44 |
| 13:YC:554[F]:MET:HE3 | 13:YC:554[F]:MET:HB3 | 1.87 | 0.44 |
| 14:YD:308[B]:ALA:O | 14:YD:357[B]:MET:N | 2.51 | 0.44 |
| 14:YD:308[F]:ALA:O | 14:YD:357[F]:MET:N | 2.51 | 0.44 |
| 14:YD:44[B]:LEU:HB2 | 14:YD:340[B]:ASP:O | 2.18 | 0.44 |
| 14:YD:73[C]:SER:HA | 14:YD:85[C]:THR:HA | 2.00 | 0.44 |
| 14:YD:88[F]:TYR:HD1 | 14:YD:110[F]:GLY:C | 2.21 | 0.44 |
| 14:YE:88[E]:TYR:HD1 | 14:YE:110[E]:GLY:C | 2.22 | 0.44 |
| 14:YE:140[B]:TYR:HE2 | 14:YE:148[B]:PRO:HD3 | 1.83 | 0.44 |
| 13:YB:26[C]:ARG:HD3 | 14:YE:259[C]:LEU:CD2 | 2.47 | 0.44 |
| 14:YE:44[A]:LEU:HB2 | 14:YE:340[A]:ASP:O | 2.18 | 0.44 |
| 14:YE:44[B]:LEU:HB2 | 14:YE:340[B]:ASP:O | 2.18 | 0.44 |
| 14:YF:132[D]:ILE:HD12 | 14:YF:197[D]:MET:SD | 2.58 | 0.44 |
| 14:YF:233[D]:ASP:OD1 | 14:YF:233[D]:ASP:N | 2.51 | 0.44 |
| 14:YF:308[B]:ALA:O | 14:YF:357[B]:MET:N | 2.51 | 0.44 |
| 14:YF:288[D]:TYR:CE1 | 14:YF:371[D]:LYS:HD3 | 2.53 | 0.44 |
| 2:Z:145:ALA:HB2 | 2:Z:542:THR:CB | 2.48 | 0.44 |
| 2:Z:336:ILE:HG21 | 2:Z:350:PHE:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:338:PHE:CE2 | 2:Z:342:SER:O | 2.69 | 0.44 |
| 2:Z:84:THR:O | 2:Z:91:GLN:NE2 | 2.51 | 0.44 |
| 2:Z:927:THR:HB | 2:Z:987:ARG:HA | 2.00 | 0.44 |
| 15:ZA:26[E]:GLN:NE2 | 15:ZA:29[E]:VAL:H | 1.93 | 0.44 |
| 1:A:116:ASP:OD1 | 1:A:118:LEU:N | 2.46 | 0.43 |
| 5:AC:149:LYS:HB2 | 5:AD:153:LYS:HZ3 | 1.83 | 0.43 |
| 5:AC:384:THR:O | 5:AC:385:TRP:HD1 | 2.01 | 0.43 |
| 5:AC:89:TYR:CE1 | 5:AC:137:TYR:CZ | 3.06 | 0.43 |
| 5:AD:177:PHE:HD2 | 5:AD:230:ILE:HD11 | 1.83 | 0.43 |
| 5:AE:316:ILE:HD11 | 6:AF:7:LYS:HZ1 | 1.83 | 0.43 |
| 6:AF:130:ARG:O | 6:AF:134:GLN:HG3 | 2.18 | 0.43 |
| 6:AG:91:SER:OG | 6:AG:177:THR:HB | 2.18 | 0.43 |
| 7:AI:26:PRO:HA | 7:AI:27:PRO:HD3 | 1.80 | 0.43 |
| 7:AI:447:HIS:CE1 | 7:BA:445:HIS:NE2 | 2.84 | 0.43 |
| 7:AJ:354:LEU:HD21 | 7:AJ:522:ILE:HG21 | 2.00 | 0.43 |
| 1:B:167:LEU:HA | 1:B:167:LEU:HD23 | 1.85 | 0.43 |
| 1:B:358:GLN:HB2 | 1:B:379:LYS:HD3 | 1.99 | 0.43 |
| 1:B:485:VAL:HG22 | 1:B:624:TYR:HD1 | 1.83 | 0.43 |
| 7:AJ:117:THR:HB | 7:BA:112:ASN:HA | 2.00 | 0.43 |
| 7:BA:197:ALA:O | 7:BA:201:GLN:HG3 | 2.18 | 0.43 |
| 7:AI:492:PRO:HD2 | 7:BA:464:ARG:NH2 | 2.32 | 0.43 |
| 10:BE:286:VAL:HG22 | 10:BE:287:VAL:N | 2.32 | 0.43 |
| 12:BG:221:ILE:HA | 12:BG:221:ILE:HD12 | 1.80 | 0.43 |
| 2:BJ:135:VAL:HG12 | 2:BJ:589:LYS:HE3 | 2.00 | 0.43 |
| 2:BJ:613:LYS:HG3 | 2:BJ:614:PRO:HD3 | 2.00 | 0.43 |
| 2:BJ:724:ALA:O | 2:BJ:725:ARG:HG2 | 2.17 | 0.43 |
| 2:BJ:819:ARG:O | 2:BJ:820:LEU:HD23 | 2.17 | 0.43 |
| 2:BJ:952:ILE:HG13 | 2:BJ:952:ILE:H | 1.47 | 0.43 |
| 2:C:420:THR:OG1 | 2:C:422:GLU:N | 2.51 | 0.43 |
| 2:C:777:LEU:HD23 | 2:C:809:TRP:CD2 | 2.53 | 0.43 |
| 3:CA:92:ARG:HD3 | 3:CA:205:ASN:O | 2.18 | 0.43 |
| 5:CF:149:LYS:HB2 | 5:CG:153:LYS:HZ3 | 1.83 | 0.43 |
| 5:CF:384:THR:O | 5:CF:385:TRP:HD1 | 2.01 | 0.43 |
| 5:CG:302:GLU:HB3 | 5:CG:365:ILE:CD1 | 2.47 | 0.43 |
| 5:CG:68:TYR:HB2 | 5:CG:70:ILE:HD11 | 2.00 | 0.43 |
| 5:CH:357:SER:HB3 | 5:CH:358:VAL:H | 1.55 | 0.43 |
| 6:CI:73:ASN:ND2 | 6:CI:215:PHE:HE2 | 2.16 | 0.43 |
| 6:CJ:108:LEU:HD23 | 6:CJ:113:PRO:HA | 2.00 | 0.43 |
| 3:D:130:VAL:HG21 | 3:D:192:PHE:CZ | 2.53 | 0.43 |
| 2:C:911:THR:HG23 | 3:D:330:ILE:HG12 | 1.99 | 0.43 |
| 2:C:1020:ARG:NH2 | 3:D:94:ASP:OD2 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:CJ:44:ALA:HA | 6:DA:110:PHE:C | 2.38 | 0.43 |
| 7:DB:59:PHE:HB2 | 7:DB:74:LYS:HG2 | 1.99 | 0.43 |
| 7:DB:60:ILE:HG22 | 7:DC:52:SER:N | 2.34 | 0.43 |
| 7:DD:197:ALA:O | 7:DD:201:GLN:HG3 | 2.18 | 0.43 |
| 8:DE:88:TRP:CE3 | 8:DE:134:PRO:HD3 | 2.53 | 0.43 |
| 8:DF:88:TRP:CE3 | 8:DF:134:PRO:HD3 | 2.53 | 0.43 |
| 3:D:16:PHE:HB2 | 3:E:310:ILE:HB | 2.00 | 0.43 |
| 1:EA:413:TYR:CE1 | 1:EA:415:PHE:HE1 | 2.36 | 0.43 |
| 1:EA:485:VAL:HG22 | 1:EA:624:TYR:CD1 | 2.53 | 0.43 |
| 1:EA:525:ASN:HB3 | 1:EA:528:THR:CG2 | 2.48 | 0.43 |
| 1:EA:561:GLY:H | 1:EA:588:LYS:NZ | 2.16 | 0.43 |
| 1:EB:276:ASN:HB2 | 1:EB:279:ASP:OD2 | 2.18 | 0.43 |
| 1:EB:351:GLU:OE1 | 1:EB:351:GLU:N | 2.48 | 0.43 |
| 1:EB:521:ARG:HB2 | 1:EB:533:ASP:CG | 2.39 | 0.43 |
| 1:EB:559:ALA:HB3 | 1:EB:562:ASP:OD2 | 2.18 | 0.43 |
| 1:EA:67:ILE:HD11 | 1:EB:67:ILE:HG21 | 2.00 | 0.43 |
| 2:EC:152:GLN:OE1 | 2:EC:152:GLN:N | 2.31 | 0.43 |
| 2:EC:213:ASN:HB2 | 2:EC:289:PHE:CZ | 2.53 | 0.43 |
| 2:EC:52:ASN:O | 2:EC:54:TYR:N | 2.51 | 0.43 |
| 3:ED:147:LEU:HD23 | 3:ED:149:ASP:N | 2.30 | 0.43 |
| 2:EC:1020:ARG:NH2 | 3:ED:94:ASP:OD2 | 2.51 | 0.43 |
| 3:EE:79:VAL:HG12 | 3:EE:80:LYS:O | 2.18 | 0.43 |
| 4:EG:107:VAL:O | 4:EG:148:LEU:N | 2.39 | 0.43 |
| 5:EI:272:SER:OG | 6:FB:106:THR:N | 2.51 | 0.43 |
| 5:EI:384:THR:O | 5:EI:385:TRP:HD1 | 2.01 | 0.43 |
| 5:EJ:177:PHE:HD2 | 5:EJ:230:ILE:HD11 | 1.83 | 0.43 |
| 5:EJ:258:TYR:CD2 | 5:EJ:259:THR:N | 2.86 | 0.43 |
| 5:EJ:322:GLY:N | 5:EJ:360:THR:HG23 | 2.33 | 0.43 |
| 5:FA:199:GLU:HG3 | 5:FA:200:LEU:N | 2.32 | 0.43 |
| 5:FA:309:LEU:HD23 | 5:FA:310:GLU:N | 2.33 | 0.43 |
| 5:EI:555:CYS:O | 5:FA:557:TYR:HE1 | 2.00 | 0.43 |
| 7:FG:12:GLU:HG3 | 7:FG:15:TYR:H | 1.82 | 0.43 |
| 7:FG:161:THR:H | 7:FG:164:LYS:HB2 | 1.83 | 0.43 |
| 8:BB:55:ASN:HD22 | 8:FH:99:ILE:HD11 | 1.82 | 0.43 |
| 11:GB:73:LEU:HD22 | 11:GB:86:TRP:CH2 | 2.52 | 0.43 |
| 11:GB:88:THR:HG22 | 11:GB:92:ALA:HB3 | 1.99 | 0.43 |
| 12:GC:195:VAL:O | 12:GC:195:VAL:HG12 | 2.16 | 0.43 |
| 1:GD:209:TRP:HD1 | 1:GD:225:TYR:CE1 | 2.35 | 0.43 |
| 1:GD:236:PHE:CD1 | 1:GD:236:PHE:N | 2.84 | 0.43 |
| 1:GD:525:ASN:HB3 | 1:GD:528:THR:CG2 | 2.48 | 0.43 |
| 1:GE:205:GLU:C | 1:GE:206:TRP:HD1 | 2.21 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:478:GLU:HG3 | 2:GF:488:MET:SD | 2.58 | 0.43 |
| 2:GF:724:ALA:C | 2:GF:726:PHE:H | 2.20 | 0.43 |
| 2:GF:37:GLU:O | 2:GF:80:ILE:HA | 2.17 | 0.43 |
| 4:GI:111:ASN:HB2 | 4:GI:116:ILE:HD12 | 1.98 | 0.43 |
| 4:GI:173:SER:N | 4:GJ:166:SER:OG | 2.39 | 0.43 |
| 4:H:145:LYS:N | 4:H:165:GLU:O | 2.49 | 0.43 |
| 4:GI:4:GLN:NE2 | 4:HA:61:ILE:O | 2.45 | 0.43 |
| 5:HB:275:SER:HA | 5:HB:280:ILE:HG22 | 2.00 | 0.43 |
| 5:HB:317:LEU:HD13 | 5:HC:312:ARG:NH1 | 2.32 | 0.43 |
| 5:HB:569:TYR:HB2 | 5:HC:550:VAL:HB | 2.00 | 0.43 |
| 6:HF:73:ASN:ND2 | 6:HF:215:PHE:HE2 | 2.16 | 0.43 |
| 7:HH:94:VAL:HG12 | 7:HH:95:TYR:O | 2.18 | 0.43 |
| 7:HI:12:GLU:CG | 7:HI:15:TYR:H | 2.31 | 0.43 |
| 7:HI:198:GLN:HA | 7:HI:201:GLN:CD | 2.38 | 0.43 |
| 7:HH:17:LYS:H | 7:HJ:11:ASN:HB2 | 1.83 | 0.43 |
| 7:HH:448:ALA:HA | 7:HJ:483:PHE:HA | 2.00 | 0.43 |
| 5:I:312:ARG:HG2 | 5:I:317:LEU:CA | 2.44 | 0.43 |
| 5:I:323:THR:CG2 | 5:I:354:THR:HG23 | 2.48 | 0.43 |
| 8:IA:5:ASP:HA | 8:IA:8:ARG:HB3 | 2.00 | 0.43 |
| 8:IA:3:VAL:HG12 | 8:IB:58:ILE:HG23 | 1.99 | 0.43 |
| 8:IB:5:ASP:HA | 8:IB:8:ARG:HB3 | 2.00 | 0.43 |
| 5:J:322:GLY:N | 5:J:360:THR:HG23 | 2.33 | 0.43 |
| 5:K:469:PRO:HD3 | 5:K:598:TRP:CE2 | 2.53 | 0.43 |
| 7:O:94:VAL:HG12 | 7:O:95:TYR:O | 2.18 | 0.43 |
| 7:Q:493:GLU:HA | 7:Q:496:ARG:NH2 | 2.32 | 0.43 |
| 8:S:5:ASP:HA | 8:S:8:ARG:HB3 | 2.00 | 0.43 |
| 10:U:225:ILE:HD13 | 10:U:225:ILE:HG21 | 1.77 | 0.43 |
| 10:U:237:THR:HA | 10:U:287:VAL:CG2 | 2.47 | 0.43 |
| 11:V:43:TYR:CE2 | 11:V:180:PHE:HB2 | 2.49 | 0.43 |
| 12:W:118:TYR:CG | 12:W:119:ASN:N | 2.86 | 0.43 |
| 1:X:123:ILE:HD11 | 1:X:295:ILE:HD11 | 2.00 | 0.43 |
| 1:X:288:TYR:CE2 | 1:X:290:ASP:O | 2.70 | 0.43 |
| 1:X:34:ILE:HG23 | 1:X:48:PHE:CD2 | 2.49 | 0.43 |
| 1:Y:373:PHE:O | 1:Y:374:ILE:HD13 | 2.18 | 0.43 |
| 13:YA:261[E]:LYS:HE2 | 13:YA:293[E]:ASN:HB3 | 1.99 | 0.43 |
| 13:YA:471[B]:LEU:O | 13:YB:463[B]:ILE:HA | 2.18 | 0.43 |
| 13:YA:521[D]:LEU:HD12 | 13:YA:522[D]:VAL:N | 2.32 | 0.43 |
| 13:YA:554[D]:MET:HE3 | 13:YA:554[D]:MET:HB3 | 1.87 | 0.43 |
| 13:YA:8[E]:LEU:HD23 | 13:YA:8[E]:LEU:HA | 1.79 | 0.43 |
| 13:YB:109[B]:ASN:OD1 | 13:YB:110[B]:ARG:N | 2.51 | 0.43 |
| 13:YB:109[F]:ASN:OD1 | 13:YB:110[F]:ARG:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:131[E]:VAL:O | 13:YB:134[E]:GLN:N | 2.46 | 0.43 |
| 13:YB:263[A]:GLY:N | 13:YB:264[A]:PRO:HD2 | 2.33 | 0.43 |
| 13:YB:389[C]:TYR:O | 13:YB:405[C]:ASP:HB2 | 2.18 | 0.43 |
| 13:YA:71[C]:GLY:HA2 | 13:YB:393[C]:MET:HA | 1.98 | 0.43 |
| 13:YC:200[F]:ILE:HD13 | 13:YC:236[F]:ILE:HD12 | 2.00 | 0.43 |
| 13:YC:257[B]:LYS:HE2 | 13:YC:266[B]:TRP:CH2 | 2.53 | 0.43 |
| 13:YC:257[D]:LYS:HE2 | 13:YC:266[D]:TRP:CH2 | 2.53 | 0.43 |
| 13:YC:261[B]:LYS:HE2 | 13:YC:293[B]:ASN:HB3 | 1.99 | 0.43 |
| 13:YC:330[C]:ILE:HD12 | 13:YC:336[C]:LEU:HD12 | 2.00 | 0.43 |
| 13:YC:36[B]:PRO:HB2 | 13:YC:38[B]:GLN:OE1 | 2.18 | 0.43 |
| 13:YC:36[E]:PRO:HB2 | 13:YC:38[E]:GLN:OE1 | 2.18 | 0.43 |
| 13:YC:47[F]:ILE:HG23 | 14:YF:123[F]:PRO:CG | 2.48 | 0.43 |
| 13:YC:490[C]:VAL:HG12 | 13:YC:492[C]:GLY:H | 1.81 | 0.43 |
| 13:YC:552[B]:GLU:CG | 13:YC:554[B]:MET:HE1 | 2.48 | 0.43 |
| 13:YC:76[A]:PRO:HG3 | 13:YC:96[A]:VAL:CG1 | 2.48 | 0.43 |
| 14:YD:127[F]:ASP:CG | 14:YD:130[F]:GLU:H | 2.20 | 0.43 |
| 14:YD:132[D]:ILE:HD12 | 14:YD:197[D]:MET:SD | 2.58 | 0.43 |
| 14:YD:132[B]:ILE:HD12 | 14:YD:197[B]:MET:SD | 2.58 | 0.43 |
| 11:DI:175:SER:HA | 14:YD:217[D]:SER:HB2 | 1.98 | 0.43 |
| 14:YD:233[E]:ASP:OD1 | 14:YD:233[E]:ASP:N | 2.51 | 0.43 |
| 14:YD:307[F]:TYR:HA | 14:YD:307[F]:TYR:HD1 | 1.66 | 0.43 |
| 14:YD:44[D]:LEU:HB2 | 14:YD:340[D]:ASP:O | 2.18 | 0.43 |
| 14:YD:308[E]:ALA:O | 14:YD:357[E]:MET:N | 2.51 | 0.43 |
| 14:YD:88[D]:TYR:HD1 | 14:YD:110[D]:GLY:C | 2.21 | 0.43 |
| 14:YE:88[B]:TYR:HD1 | 14:YE:110[B]:GLY:C | 2.21 | 0.43 |
| 14:YF:109[F]:LEU:HA | 14:YF:109[F]:LEU:HD12 | 1.65 | 0.43 |
| 14:YF:132[C]:ILE:HD12 | 14:YF:197[C]:MET:SD | 2.58 | 0.43 |
| 14:YF:233[A]:ASP:OD1 | 14:YF:233[A]:ASP:N | 2.51 | 0.43 |
| 14:YF:233[F]:ASP:N | 14:YF:233[F]:ASP:OD1 | 2.51 | 0.43 |
| 14:YD:91[B]:LYS:O | 14:YF:242[B]:PRO:HD2 | 2.18 | 0.43 |
| 14:YF:288[B]:TYR:CE1 | 14:YF:371[B]:LYS:HD3 | 2.53 | 0.43 |
| 14:YF:288[E]:TYR:CE1 | 14:YF:371[E]:LYS:HD3 | 2.52 | 0.43 |
| 14:YF:38[F]:LEU:HA | 14:YF:38[F]:LEU:HD12 | 1.63 | 0.43 |
| 14:YF:44[C]:LEU:HB2 | 14:YF:340[C]:ASP:O | 2.18 | 0.43 |
| 14:YF:44[D]:LEU:HB2 | 14:YF:340[D]:ASP:O | 2.18 | 0.43 |
| 14:YF:44[F]:LEU:HB2 | 14:YF:340[F]:ASP:O | 2.18 | 0.43 |
| 5:AC:103:ASN:O | 5:AC:104:VAL:C | 2.56 | 0.43 |
| 5:AC:166:GLU:N | 5:AC:166:GLU:OE1 | 2.52 | 0.43 |
| 5:AC:285:LEU:HD11 | 5:AC:375:PHE:CB | 2.41 | 0.43 |
| 5:AC:302:GLU:HG3 | 5:AC:303:PRO:HD2 | 2.00 | 0.43 |
| 5:AC:323:THR:HG21 | 5:AC:354:THR:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:402:GLU:HG2 | 5:AE:396:LYS:HE3 | 1.99 | 0.43 |
| 5:AC:49:TRP:HZ3 | 5:AC:96:ARG:HD2 | 1.80 | 0.43 |
| 5:AC:502:ASN:OD1 | 5:AC:504:ASN:N | 2.51 | 0.43 |
| 5:AD:322:GLY:O | 5:AD:323:THR:OG1 | 2.33 | 0.43 |
| 5:AD:323:THR:HG22 | 5:AD:355:ASP:O | 2.18 | 0.43 |
| 5:AD:569:TYR:HD1 | 5:AE:544:VAL:HA | 1.84 | 0.43 |
| 5:AE:377:HIS:CG | 5:AE:378:GLY:N | 2.85 | 0.43 |
| 5:AE:469:PRO:HD3 | 5:AE:598:TRP:CE2 | 2.53 | 0.43 |
| 5:AC:416:ILE:HG23 | 5:AE:472:TYR:HA | 2.00 | 0.43 |
| 6:AF:91:SER:OG | 6:AF:177:THR:HB | 2.18 | 0.43 |
| 7:AI:17:LYS:H | 7:BA:11:ASN:HB2 | 1.83 | 0.43 |
| 7:AI:299:THR:O | 7:BA:293:GLY:N | 2.50 | 0.43 |
| 7:AI:329:ASN:OD1 | 7:AI:330:ARG:N | 2.50 | 0.43 |
| 7:AJ:116:ILE:HG23 | 7:AJ:120:LYS:HB2 | 2.00 | 0.43 |
| 7:AI:161:THR:HA | 7:AJ:158:THR:O | 2.17 | 0.43 |
| 1:B:199:LEU:HD21 | 1:B:224:TYR:CG | 2.53 | 0.43 |
| 1:B:485:VAL:HG11 | 1:B:650:TYR:CE1 | 2.53 | 0.43 |
| 8:BC:5:ASP:HA | 8:BC:8:ARG:HB3 | 2.00 | 0.43 |
| 12:BG:112:ASP:O | 12:BG:116:MET:N | 2.41 | 0.43 |
| 12:BG:8:ASN:HA | 12:BG:12:ILE:HG22 | 2.00 | 0.43 |
| 2:BJ:494:GLU:HG3 | 2:BJ:498:TRP:CG | 2.53 | 0.43 |
| 1:BH:60:LEU:HD13 | 2:BJ:671:TYR:CD1 | 2.53 | 0.43 |
| 2:C:479:TRP:H | 2:C:479:TRP:HE3 | 1.64 | 0.43 |
| 2:C:494:GLU:HG3 | 2:C:498:TRP:CG | 2.53 | 0.43 |
| 2:C:572:ASN:CB | 2:C:611:ILE:HG22 | 2.48 | 0.43 |
| 2:C:855:ILE:HA | 2:C:855:ILE:HD12 | 1.86 | 0.43 |
| 2:C:883:VAL:HG13 | 2:C:884:HIS:H | 1.82 | 0.43 |
| 4:CD:192:PHE:CE1 | 4:CD:197:TYR:HB2 | 2.53 | 0.43 |
| 5:CF:166:GLU:N | 5:CF:166:GLU:OE1 | 2.52 | 0.43 |
| 5:CF:213:GLY:CA | 5:CF:221:GLU:HB2 | 2.47 | 0.43 |
| 5:CF:262:GLN:HA | 5:CF:381:ILE:O | 2.17 | 0.43 |
| 5:CF:288:MET:HG2 | 5:CF:289:LYS:O | 2.18 | 0.43 |
| 5:CF:502:ASN:OD1 | 5:CF:504:ASN:N | 2.51 | 0.43 |
| 5:CF:571:GLU:OE2 | 5:CH:567:THR:HG21 | 2.18 | 0.43 |
| 5:CG:275:SER:OG | 5:CG:281:TYR:HA | 2.19 | 0.43 |
| 5:CF:317:LEU:HD13 | 5:CG:312:ARG:NH2 | 2.32 | 0.43 |
| 5:CF:569:TYR:HB2 | 5:CG:550:VAL:HB | 2.00 | 0.43 |
| 5:CH:199:GLU:HG3 | 5:CH:200:LEU:N | 2.32 | 0.43 |
| 6:CI:199:GLN:HB2 | 6:CJ:203:LEU:CD2 | 2.48 | 0.43 |
| 3:D:128:TRP:HB2 | 3:D:194:ILE:HB | 1.99 | 0.43 |
| 7:DB:65:GLU:O | 7:DB:69:GLY:N | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DC:116:ILE:HG23 | 7:DC:120:LYS:HB2 | 2.00 | 0.43 |
| 7:DC:129:PHE:CE2 | 7:DC:141:VAL:HG11 | 2.52 | 0.43 |
| 7:DC:40:SER:HB3 | 7:DD:24:ASN:CB | 2.47 | 0.43 |
| 7:DD:413:ASN:O | 7:DD:424:ARG:HD3 | 2.17 | 0.43 |
| 8:DF:61:ALA:HB2 | 8:FI:133:TRP:CH2 | 2.53 | 0.43 |
| 9:DG:10:ASP:O | 9:DG:26:SER:N | 2.48 | 0.43 |
| 11:DI:2:LEU:HD23 | 11:DI:32:TYR:CD1 | 2.53 | 0.43 |
| 3:E:106:PHE:CD2 | 3:E:188:TRP:HH2 | 2.35 | 0.43 |
| 3:E:178:GLY:O | 3:E:180:ILE:N | 2.51 | 0.43 |
| 1:EA:167:LEU:HA | 1:EA:167:LEU:HD23 | 1.76 | 0.43 |
| 1:EA:446:ARG:NE | 1:EA:450:GLU:OE2 | 2.51 | 0.43 |
| 1:EB:341:THR:OG1 | 1:EB:342:ALA:N | 2.51 | 0.43 |
| 2:EC:420:THR:OG1 | 2:EC:422:GLU:N | 2.51 | 0.43 |
| 2:EC:455:VAL:CG2 | 2:EC:472:LYS:HB3 | 2.49 | 0.43 |
| 3:ED:16:PHE:HB2 | 3:EE:310:ILE:HB | 2.00 | 0.43 |
| 4:EF:192:PHE:CE1 | 4:EF:197:TYR:HB2 | 2.53 | 0.43 |
| 4:EG:152:SER:O | 4:EG:158:SER:HA | 2.18 | 0.43 |
| 4:EF:172:GLU:OE1 | 4:EG:164:ILE:HG23 | 2.17 | 0.43 |
| 5:EI:180:VAL:HG22 | 5:EI:181:PHE:H | 1.83 | 0.43 |
| 5:EI:267:ASP:CG | 5:EI:285:LEU:HB2 | 2.38 | 0.43 |
| 5:EI:421:ASN:HB2 | 5:EI:434:GLU:CG | 2.47 | 0.43 |
| 5:EJ:323:THR:HB | 5:EJ:355:ASP:HB3 | 1.99 | 0.43 |
| 5:FA:207:SER:O | 5:FA:210:SER:OG | 2.32 | 0.43 |
| 6:FC:73:ASN:ND2 | 6:FC:215:PHE:HE2 | 2.16 | 0.43 |
| 6:FD:88:TRP:O | 6:FD:155:LYS:HA | 2.18 | 0.43 |
| 7:FE:453:GLU:CD | 7:FE:471:THR:H | 2.18 | 0.43 |
| 7:FF:248:ALA:O | 7:FF:252:GLY:N | 2.47 | 0.43 |
| 7:FG:134:SER:HB3 | 7:FG:140:GLY:N | 2.33 | 0.43 |
| 7:FG:272:GLN:NE2 | 7:FG:277:ALA:HA | 2.33 | 0.43 |
| 7:FG:407:SER:HA | 7:FG:410:THR:OG1 | 2.17 | 0.43 |
| 8:FH:5:ASP:HA | 8:FH:8:ARG:HB3 | 2.00 | 0.43 |
| 8:FI:88:TRP:CE3 | 8:FI:134:PRO:HD3 | 2.53 | 0.43 |
| 11:GB:44:ARG:HG2 | 11:GB:45:LEU:N | 2.33 | 0.43 |
| 12:GC:164:MET:HB3 | 12:GC:237:THR:HG22 | 2.01 | 0.43 |
| 1:GD:365:ASP:OD2 | 1:GD:367:THR:HB | 2.18 | 0.43 |
| 1:GD:523:VAL:O | 1:GD:531:GLU:HB2 | 2.18 | 0.43 |
| 1:GE:206:TRP:CG | 1:GE:222:THR:HB | 2.53 | 0.43 |
| 1:GE:358:GLN:HB2 | 1:GE:379:LYS:HD3 | 1.99 | 0.43 |
| 2:GF:160:VAL:O | 2:GF:163:ILE:HB | 2.18 | 0.43 |
| 2:GF:572:ASN:CB | 2:GF:611:ILE:HG22 | 2.48 | 0.43 |
| 2:GF:819:ARG:O | 2:GF:820:LEU:HD23 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:448:PHE:CE2 | 3:GG:66:LEU:HD11 | 2.53 | 0.43 |
| 4:GJ:67:TYR:CE1 | 4:GJ:84:ARG:HD3 | 2.52 | 0.43 |
| 4:H:28:GLY:O | 4:H:32:ASN:ND2 | 2.51 | 0.43 |
| 5:HB:229:ASN:OD1 | 5:HB:230:ILE:N | 2.51 | 0.43 |
| 5:HB:502:ASN:OD1 | 5:HB:504:ASN:N | 2.51 | 0.43 |
| 5:HC:177:PHE:HD2 | 5:HC:230:ILE:HD11 | 1.83 | 0.43 |
| 5:HC:323:THR:HG22 | 5:HC:355:ASP:O | 2.18 | 0.43 |
| 5:HC:322:GLY:N | 5:HC:360:THR:HG23 | 2.33 | 0.43 |
| 5:HD:137:TYR:HA | 5:HD:143:TRP:HD1 | 1.81 | 0.43 |
| 5:HB:255:ARG:NH2 | 5:HD:390:LEU:HB2 | 2.32 | 0.43 |
| 5:HC:569:TYR:CE1 | 5:HD:544:VAL:HG22 | 2.52 | 0.43 |
| 5:HD:469:PRO:HD3 | 5:HD:598:TRP:CE2 | 2.53 | 0.43 |
| 5:HD:69:ALA:HB1 | 5:HD:98:VAL:HG23 | 1.99 | 0.43 |
| 6:HE:86:ASP:CG | 6:HE:180:GLN:HE21 | 2.19 | 0.43 |
| 6:HE:32:ARG:NH1 | 6:HF:144:ASN:OD1 | 2.45 | 0.43 |
| 7:HH:276:ASP:OD1 | 7:HI:260:ARG:NH2 | 2.50 | 0.43 |
| 7:HH:77:THR:HG22 | 7:HH:80:THR:H | 1.83 | 0.43 |
| 7:HI:129:PHE:CE2 | 7:HI:141:VAL:HG11 | 2.52 | 0.43 |
| 7:HJ:134:SER:HB3 | 7:HJ:140:GLY:N | 2.33 | 0.43 |
| 7:HJ:12:GLU:HG3 | 7:HJ:15:TYR:H | 1.83 | 0.43 |
| 7:HJ:218:SER:O | 7:HJ:227:VAL:HG22 | 2.19 | 0.43 |
| 7:HJ:228:ILE:HG22 | 7:HJ:229:LYS:N | 2.33 | 0.43 |
| 5:I:329:PHE:HB3 | 5:I:332:VAL:CB | 2.42 | 0.43 |
| 5:I:421:ASN:HB2 | 5:I:434:GLU:CG | 2.47 | 0.43 |
| 5:I:89:TYR:CE1 | 5:I:137:TYR:CZ | 3.06 | 0.43 |
| 9:IC:33:LYS:HG2 | 9:IC:122:ILE:HG21 | 1.99 | 0.43 |
| 11:IE:186:ARG:HG3 | 11:IE:187:ILE:N | 2.33 | 0.43 |
| 12:IF:118:TYR:CG | 12:IF:119:ASN:N | 2.86 | 0.43 |
| 5:J:115:ASP:OD2 | 5:J:137:TYR:HE1 | 2.01 | 0.43 |
| 5:K:117:ILE:HG13 | 5:K:118:LYS:H | 1.84 | 0.43 |
| 5:K:352:SER:HB2 | 5:K:354:THR:O | 2.18 | 0.43 |
| 5:I:571:GLU:OE2 | 5:K:567:THR:HG21 | 2.18 | 0.43 |
| 5:K:69:ALA:HB1 | 5:K:98:VAL:HG23 | 2.00 | 0.43 |
| 6:M:73:ASN:ND2 | 6:M:215:PHE:HE2 | 2.16 | 0.43 |
| 6:N:130:ARG:O | 6:N:134:GLN:HG3 | 2.18 | 0.43 |
| 5:I:318:GLN:NE2 | 6:N:4:LEU:O | 2.49 | 0.43 |
| 6:N:47:PHE:HE2 | 6:N:51:ASN:HB3 | 1.84 | 0.43 |
| 7:O:424:ARG:O | 7:P:504:ARG:NH2 | 2.50 | 0.43 |
| 7:P:12:GLU:CG | 7:P:15:TYR:H | 2.31 | 0.43 |
| 7:P:20:PRO:HB3 | 7:P:29:ILE:HG13 | 2.00 | 0.43 |
| 7:O:347:MET:HE2 | 7:P:345:ALA:HB1 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:V:107:ASP:HA | 11:V:155:THR:HG22 | 2.00 | 0.43 |
| 11:V:73:LEU:HD22 | 11:V:86:TRP:CH2 | 2.52 | 0.43 |
| 8:R:53:PHE:HB2 | 12:W:7:PHE:CE2 | 2.53 | 0.43 |
| 1:X:210:THR:CG2 | 1:X:226:MET:H | 2.31 | 0.43 |
| 1:Y:246:ASN:N | 1:Y:246:ASN:OD1 | 2.48 | 0.43 |
| 1:Y:485:VAL:HG22 | 1:Y:624:TYR:HD1 | 1.83 | 0.43 |
| 13:YA:236[A]:ILE:HG23 | 13:YA:240[A]:GLU:HB2 | 1.99 | 0.43 |
| 13:YA:257[E]:LYS:HE2 | 13:YA:266[E]:TRP:CH2 | 2.53 | 0.43 |
| 13:YA:263[A]:GLY:N | 13:YA:264[A]:PRO:HD2 | 2.33 | 0.43 |
| 13:YA:263[C]:GLY:N | 13:YA:264[C]:PRO:HD2 | 2.33 | 0.43 |
| 13:YA:263[E]:GLY:N | 13:YA:264[E]:PRO:HD2 | 2.33 | 0.43 |
| 13:YA:304[A]:TRP:O | 13:YA:308[A]:TYR:N | 2.32 | 0.43 |
| 13:YA:320[F]:THR:HG22 | 13:YA:323[F]:ARG:HB3 | 2.00 | 0.43 |
| 13:YA:330[F]:ILE:HD12 | 13:YA:336[F]:LEU:HD12 | 2.00 | 0.43 |
| 13:YA:36[E]:PRO:HB2 | 13:YA:38[E]:GLN:OE1 | 2.18 | 0.43 |
| 13:YA:376[F]:PHE:CD2 | 13:YB:447[F]:ASN:OD1 | 2.71 | 0.43 |
| 13:YA:471[C]:LEU:O | 13:YB:463[C]:ILE:HA | 2.18 | 0.43 |
| 13:YA:564[D]:GLN:HG3 | 13:YA:566[D]:THR:HG22 | 2.01 | 0.43 |
| 13:YA:565[C]:TYR:CZ | 13:YB:557[C]:MET:HG2 | 2.53 | 0.43 |
| 13:YA:76[C]:PRO:HB2 | 13:YA:97[C]:LEU:C | 2.38 | 0.43 |
| 13:YB:109[C]:ASN:OD1 | 13:YB:110[C]:ARG:N | 2.51 | 0.43 |
| 13:YB:127[F]:ASN:ND2 | 13:YB:129[F]:THR:OG1 | 2.52 | 0.43 |
| 13:YB:147[A]:ILE:HD11 | 13:YB:188[A]:LEU:HG | 2.00 | 0.43 |
| 13:YB:24[B]:LEU:HD21 | 13:YC:102[B]:GLY:HA2 | 2.01 | 0.43 |
| 13:YB:26[D]:ARG:HD3 | 14:YE:259[D]:LEU:CD2 | 2.48 | 0.43 |
| 13:YB:442[F]:THR:HB | 13:YC:434[F]:THR:HB | 2.01 | 0.43 |
| 13:YB:458[D]:VAL:HG21 | 13:YC:454[D]:LYS:HD2 | 1.99 | 0.43 |
| 13:YB:50[D]:GLU:N | 13:YB:50[D]:GLU:CD | 2.71 | 0.43 |
| 13:YB:50[E]:GLU:N | 13:YB:50[E]:GLU:CD | 2.71 | 0.43 |
| 13:YA:569[F]:GLY:HA2 | 13:YB:561[F]:SER:O | 2.18 | 0.43 |
| 13:YB:92[E]:THR:HB | 14:YE:282[E]:ALA:CB | 2.47 | 0.43 |
| 13:YC:109[B]:ASN:OD1 | 13:YC:110[B]:ARG:N | 2.51 | 0.43 |
| 13:YA:473[F]:GLN:OE1 | 13:YC:158[F]:PRO:HB2 | 2.18 | 0.43 |
| 13:YC:200[C]:ILE:HD13 | 13:YC:236[C]:ILE:HD12 | 2.01 | 0.43 |
| 13:YC:263[E]:GLY:N | 13:YC:264[E]:PRO:HD2 | 2.33 | 0.43 |
| 13:YC:320[B]:THR:HG22 | 13:YC:323[B]:ARG:HB3 | 2.00 | 0.43 |
| 13:YA:452[F]:GLY:CA | 13:YC:321[F]:LYS:HD3 | 2.40 | 0.43 |
| 13:YC:389[F]:TYR:O | 13:YC:405[F]:ASP:HB2 | 2.18 | 0.43 |
| 13:YA:452[E]:GLY:O | 13:YC:460[E]:GLY:N | 2.52 | 0.43 |
| 13:YA:544[B]:TRP:HB2 | 13:YC:552[B]:GLU:HB2 | 2.00 | 0.43 |
| 13:YA:551[D]:THR:HA | 13:YC:558[D]:SER:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:8[A]:LEU:HA | 13:YC:8[A]:LEU:HD23 | 1.79 | 0.43 |
| 14:YD:17[F]:PHE:HE2 | 14:YD:26[F]:ASN:HA | 1.83 | 0.43 |
| 14:YD:132[C]:ILE:HD12 | 14:YD:197[C]:MET:SD | 2.58 | 0.43 |
| 10:DH:285:LEU:HA | 14:YD:215[D]:GLU:CG | 2.47 | 0.43 |
| 14:YD:233[B]:ASP:OD1 | 14:YD:233[B]:ASP:N | 2.51 | 0.43 |
| 11:GB:182:ASN:ND2 | 14:YD:327[E]:ASN:HD22 | 2.16 | 0.43 |
| 14:YE:127[F]:ASP:CG | 14:YE:130[F]:GLU:H | 2.20 | 0.43 |
| 14:YE:132[F]:ILE:HD12 | 14:YE:197[F]:MET:SD | 2.59 | 0.43 |
| 11:BF:175:SER:HA | 14:YE:217[A]:SER:HB2 | 1.99 | 0.43 |
| 14:YE:44[F]:LEU:HB2 | 14:YE:340[F]:ASP:O | 2.18 | 0.43 |
| 14:YE:38[A]:LEU:HD12 | 14:YE:38[A]:LEU:HA | 1.63 | 0.43 |
| 14:YE:44[E]:LEU:HB2 | 14:YE:340[E]:ASP:O | 2.18 | 0.43 |
| 14:YF:233[C]:ASP:OD1 | 14:YF:233[C]:ASP:N | 2.51 | 0.43 |
| 14:YF:73[D]:SER:HA | 14:YF:85[D]:THR:HA | 2.01 | 0.43 |
| 14:YF:80[B]:ILE:HD13 | 14:YF:80[B]:ILE:H | 1.83 | 0.43 |
| 14:YF:80[C]:ILE:H | 14:YF:80[C]:ILE:HD13 | 1.83 | 0.43 |
| 2:Z:494:GLU:HG3 | 2:Z:498:TRP:CG | 2.53 | 0.43 |
| 1:X:60:LEU:HD13 | 2:Z:671:TYR:CD1 | 2.53 | 0.43 |
| 2:Z:777:LEU:HD23 | 2:Z:809:TRP:CD2 | 2.53 | 0.43 |
| 1:A:157:LYS:O | 1:A:158:ASN:CG | 2.57 | 0.43 |
| 1:A:172:ILE:HD13 | 1:A:273:ILE:HG12 | 1.99 | 0.43 |
| 1:A:446:ARG:NE | 1:A:450:GLU:OE2 | 2.51 | 0.43 |
| 1:A:525:ASN:HB3 | 1:A:528:THR:CG2 | 2.48 | 0.43 |
| 5:AC:193:VAL:O | 5:AC:199:GLU:N | 2.46 | 0.43 |
| 5:AC:195:HIS:NE2 | 5:AC:236:CYS:SG | 2.85 | 0.43 |
| 5:AC:248:MET:HB2 | 5:AC:254:TRP:CD1 | 2.52 | 0.43 |
| 5:AC:275:SER:OG | 5:AC:281:TYR:HA | 2.18 | 0.43 |
| 5:AC:394:LEU:HD22 | 5:AE:395:THR:HA | 2.00 | 0.43 |
| 5:AE:309:LEU:HD23 | 5:AE:310:GLU:N | 2.33 | 0.43 |
| 5:AE:357:SER:HA | 5:AE:371:PHE:CD1 | 2.54 | 0.43 |
| 5:AC:535:THR:OG1 | 5:AE:576:THR:HB | 2.18 | 0.43 |
| 5:AC:49:TRP:C | 5:AE:90:ASN:HD21 | 2.11 | 0.43 |
| 6:AG:71:ILE:O | 6:AG:215:PHE:N | 2.36 | 0.43 |
| 7:AI:255:SER:O | 7:AI:278:SER:OG | 2.29 | 0.43 |
| 7:BA:228:ILE:HG22 | 7:BA:229:LYS:N | 2.33 | 0.43 |
| 1:BH:559:ALA:N | 1:BH:586:ARG:HD2 | 2.34 | 0.43 |
| 1:BI:451:ASP:O | 1:BI:454:ILE:HD12 | 2.17 | 0.43 |
| 2:BJ:114:ILE:HG23 | 2:BJ:115:GLU:N | 2.33 | 0.43 |
| 1:BI:610:ASN:ND2 | 2:BJ:804:ASN:HA | 2.33 | 0.43 |
| 2:BJ:878:ASP:O | 2:BJ:881:ARG:N | 2.49 | 0.43 |
| 2:BJ:948:THR:HB | 2:BJ:950:GLU:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:404:TYR:CE1 | 2:C:415:ARG:HG2 | 2.54 | 0.43 |
| 2:C:725:ARG:HA | 2:C:728:GLU:HB3 | 2.00 | 0.43 |
| 2:C:84:THR:O | 2:C:91:GLN:NE2 | 2.51 | 0.43 |
| 3:CA:150:LYS:HA | 3:CA:160:TRP:CZ3 | 2.53 | 0.43 |
| 5:CF:180:VAL:HG22 | 5:CF:181:PHE:H | 1.84 | 0.43 |
| 5:CF:193:VAL:O | 5:CF:199:GLU:N | 2.46 | 0.43 |
| 5:CF:22:GLY:O | 5:CF:26:ILE:N | 2.37 | 0.43 |
| 5:CF:323:THR:CG2 | 5:CF:359:GLU:HB2 | 2.48 | 0.43 |
| 5:CG:322:GLY:N | 5:CG:360:THR:HG23 | 2.33 | 0.43 |
| 6:CI:144:ASN:HB3 | 6:CI:159:THR:HG22 | 1.99 | 0.43 |
| 6:CI:47:PHE:HE2 | 6:CI:51:ASN:HB3 | 1.84 | 0.43 |
| 6:CJ:172:SER:HA | 6:CJ:176:ILE:O | 2.17 | 0.43 |
| 6:DA:130:ARG:O | 6:DA:134:GLN:HG3 | 2.18 | 0.43 |
| 6:CJ:10:VAL:CA | 6:DA:13:ARG:HD2 | 2.32 | 0.43 |
| 7:DB:130:GLU:OE2 | 7:DC:132:ARG:NH1 | 2.37 | 0.43 |
| 7:DB:228:ILE:O | 7:DC:225:LYS:HA | 2.18 | 0.43 |
| 7:DB:485:ASN:OD1 | 7:DD:448:ALA:N | 2.51 | 0.43 |
| 7:DC:126:ASN:O | 7:DC:129:PHE:HB3 | 2.18 | 0.43 |
| 7:DD:12:GLU:HG3 | 7:DD:15:TYR:H | 1.82 | 0.43 |
| 1:BH:52:ARG:HH21 | 9:DG:25:ARG:HB3 | 1.83 | 0.43 |
| 3:E:140:GLY:HA2 | 3:E:163:SER:N | 2.33 | 0.43 |
| 3:D:289:ASN:ND2 | 3:E:233:GLN:HB2 | 2.33 | 0.43 |
| 1:EA:559:ALA:N | 1:EA:586:ARG:HD2 | 2.33 | 0.43 |
| 1:EB:199:LEU:HD21 | 1:EB:224:TYR:CG | 2.53 | 0.43 |
| 2:EC:186:ASP:HB3 | 2:EC:189:ARG:HE | 1.83 | 0.43 |
| 2:EC:777:LEU:HD23 | 2:EC:809:TRP:CD2 | 2.53 | 0.43 |
| 2:EC:911:THR:HG23 | 3:ED:330:ILE:HG12 | 1.99 | 0.43 |
| 2:EC:948:THR:HB | 2:EC:950:GLU:OE1 | 2.18 | 0.43 |
| 4:EF:111:ASN:HB2 | 4:EF:116:ILE:HD12 | 1.98 | 0.43 |
| 5:EI:166:GLU:OE1 | 5:EI:166:GLU:N | 2.52 | 0.43 |
| 5:EI:229:ASN:OD1 | 5:EI:230:ILE:N | 2.51 | 0.43 |
| 5:EI:192:ARG:HG3 | 5:EI:245:GLU:HB2 | 1.99 | 0.43 |
| 5:EI:89:TYR:CE1 | 5:EI:137:TYR:CZ | 3.06 | 0.43 |
| 5:EJ:288:MET:HE1 | 5:EJ:292:PRO:HD3 | 1.99 | 0.43 |
| 5:EJ:491:ASN:ND2 | 5:EJ:496:ASP:HB2 | 2.27 | 0.43 |
| 5:FA:102:TRP:CZ3 | 5:FA:131:SER:HB2 | 2.53 | 0.43 |
| 6:FB:73:ASN:ND2 | 6:FB:215:PHE:HE2 | 2.16 | 0.43 |
| 5:EI:318:GLN:HE22 | 6:FD:7:LYS:HB3 | 1.82 | 0.43 |
| 7:FE:111:ASN:CG | 7:FE:114:SER:HB3 | 2.38 | 0.43 |
| 7:FE:346:ILE:HD11 | 7:FG:350:ALA:HB2 | 2.00 | 0.43 |
| 7:FE:60:ILE:HG22 | 7:FF:51:SER:C | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:28:GLY:O | 4:G:32:ASN:ND2 | 2.51 | 0.43 |
| 11:GB:36:PHE:HZ | 11:GB:76:CYS:SG | 2.40 | 0.43 |
| 2:GF:213:ASN:HB2 | 2:GF:289:PHE:CZ | 2.53 | 0.43 |
| 2:GF:584:GLY:CA | 2:GF:600:PHE:HB3 | 2.48 | 0.43 |
| 2:GF:777:LEU:HD23 | 2:GF:809:TRP:CD2 | 2.53 | 0.43 |
| 3:GG:274:ILE:HD12 | 3:GG:311:TYR:HB3 | 1.99 | 0.43 |
| 4:GI:28:GLY:O | 4:GI:32:ASN:ND2 | 2.51 | 0.43 |
| 4:GJ:67:TYR:CD1 | 4:GJ:84:ARG:HB3 | 2.50 | 0.43 |
| 5:HB:275:SER:OG | 5:HB:281:TYR:HA | 2.19 | 0.43 |
| 5:HB:312:ARG:HG2 | 5:HB:317:LEU:CA | 2.44 | 0.43 |
| 5:HC:115:ASP:OD2 | 5:HC:137:TYR:HE1 | 2.01 | 0.43 |
| 5:HB:154:ILE:HG23 | 5:HC:153:LYS:HZ1 | 1.82 | 0.43 |
| 5:HC:253:GLN:HB2 | 5:HC:255:ARG:HE | 1.84 | 0.43 |
| 5:HC:577:ASN:ND2 | 5:HD:529:ASN:OD1 | 2.39 | 0.43 |
| 6:HE:88:TRP:O | 6:HE:155:LYS:HA | 2.18 | 0.43 |
| 7:HH:246:THR:HG1 | 7:HH:249:THR:H | 1.60 | 0.43 |
| 7:HJ:182:THR:O | 7:HJ:189:GLY:HA3 | 2.18 | 0.43 |
| 7:HJ:232:THR:HG23 | 7:HJ:234:SER:N | 2.34 | 0.43 |
| 7:HH:257:THR:HA | 7:HJ:265:LEU:O | 2.18 | 0.43 |
| 5:I:160:SER:HB3 | 5:J:161:ASN:ND2 | 2.21 | 0.43 |
| 5:I:166:GLU:OE1 | 5:I:166:GLU:N | 2.52 | 0.43 |
| 5:I:186:TYR:HH | 5:I:191:ILE:HA | 1.83 | 0.43 |
| 5:I:288:MET:HG2 | 5:I:289:LYS:O | 2.18 | 0.43 |
| 8:IA:15:PHE:N | 8:IA:15:PHE:CD1 | 2.84 | 0.43 |
| 8:IA:118:ARG:HE | 8:IB:62:GLY:HA2 | 1.83 | 0.43 |
| 12:IF:8:ASN:HA | 12:IF:12:ILE:HG22 | 2.00 | 0.43 |
| 12:IF:221:ILE:HD12 | 12:IF:221:ILE:HA | 1.80 | 0.43 |
| 12:W:228:LEU:HD13 | 12:IF:22:PHE:CG | 2.54 | 0.43 |
| 5:I:518:GLY:N | 5:K:594:THR:OG1 | 2.50 | 0.43 |
| 6:L:130:ARG:O | 6:L:134:GLN:HG3 | 2.18 | 0.43 |
| 6:N:90:PHE:CD2 | 6:N:126:VAL:HG22 | 2.45 | 0.43 |
| 7:O:475:LEU:HA | 7:P:470:GLY:O | 2.17 | 0.43 |
| 7:P:110:VAL:HG12 | 7:P:111:ASN:N | 2.33 | 0.43 |
| 7:Q:228:ILE:HG22 | 7:Q:229:LYS:N | 2.33 | 0.43 |
| 7:O:288:ILE:HG13 | 7:Q:288:ILE:HG22 | 2.00 | 0.43 |
| 7:O:492:PRO:HD2 | 7:Q:464:ARG:NH2 | 2.34 | 0.43 |
| 8:S:32:PHE:O | 8:S:35:GLN:N | 2.50 | 0.43 |
| 11:V:31:ASN:O | 11:V:32:TYR:HB2 | 2.18 | 0.43 |
| 11:V:43:TYR:O | 11:V:44:ARG:HB2 | 2.19 | 0.43 |
| 1:X:432:SER:O | 1:X:435:TRP:HB3 | 2.18 | 0.43 |
| 1:Y:332:LYS:O | 1:Y:335:THR:HG22 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:340:VAL:O | 1:Y:341:THR:OG1 | 2.27 | 0.43 |
| 1:Y:352:ARG:HD2 | 1:Y:352:ARG:HA | 1.82 | 0.43 |
| 1:Y:521:ARG:HB2 | 1:Y:533:ASP:CG | 2.39 | 0.43 |
| 13:YA:109[B]:ASN:OD1 | 13:YA:110[B]:ARG:N | 2.51 | 0.43 |
| 13:YA:112[F]:GLU:C | 13:YA:115[F]:SER:HB3 | 2.39 | 0.43 |
| 13:YA:127[F]:ASN:ND2 | 13:YA:129[F]:THR:OG1 | 2.52 | 0.43 |
| 13:YA:147[C]:ILE:HD11 | 13:YA:188[C]:LEU:HG | 2.00 | 0.43 |
| 13:YA:200[B]:ILE:HD13 | 13:YA:236[B]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:47[D]:ILE:HG12 | 14:YD:123[D]:PRO:HD3 | 2.00 | 0.43 |
| 13:YA:516[D]:GLY:O | 13:YC:522[D]:VAL:HG23 | 2.17 | 0.43 |
| 13:YA:521[A]:LEU:HD12 | 13:YA:522[A]:VAL:N | 2.32 | 0.43 |
| 13:YA:58[C]:ILE:HG12 | 13:YA:97[C]:LEU:HD22 | 2.01 | 0.43 |
| 13:YB:112[C]:GLU:C | 13:YB:115[C]:SER:HB3 | 2.39 | 0.43 |
| 13:YB:112[D]:GLU:C | 13:YB:115[D]:SER:HB3 | 2.39 | 0.43 |
| 13:YB:147[C]:ILE:HD11 | 13:YB:188[C]:LEU:HG | 2.00 | 0.43 |
| 13:YB:200[B]:ILE:HD13 | 13:YB:236[B]:ILE:HD12 | 2.01 | 0.43 |
| 13:YB:200[C]:ILE:HD13 | 13:YB:236[C]:ILE:HD12 | 2.01 | 0.43 |
| 13:YB:278[A]:GLU:O | 13:YB:282[A]:PHE:N | 2.52 | 0.43 |
| 13:YB:444[F]:ALA:HB3 | 13:YC:437[F]:ASN:HA | 2.00 | 0.43 |
| 13:YB:490[E]:VAL:HG12 | 13:YB:492[E]:GLY:H | 1.81 | 0.43 |
| 13:YB:521[B]:LEU:HD12 | 13:YB:522[B]:VAL:N | 2.32 | 0.43 |
| 13:YB:552[C]:GLU:CG | 13:YB:554[C]:MET:HE1 | 2.48 | 0.43 |
| 13:YA:560[C]:ILE:O | 13:YB:553[C]:LYS:HA | 2.18 | 0.43 |
| 13:YB:8[C]:LEU:HD23 | 13:YB:8[C]:LEU:HA | 1.79 | 0.43 |
| 13:YC:109[E]:ASN:OD1 | 13:YC:110[E]:ARG:N | 2.51 | 0.43 |
| 13:YC:257[C]:LYS:HE2 | 13:YC:266[C]:TRP:CH2 | 2.52 | 0.43 |
| 13:YC:263[A]:GLY:N | 13:YC:264[A]:PRO:HD2 | 2.33 | 0.43 |
| 13:YC:263[C]:GLY:N | 13:YC:264[C]:PRO:HD2 | 2.33 | 0.43 |
| 13:YC:314[F]:SER:OG | 13:YC:316[F]:TRP:HB3 | 2.18 | 0.43 |
| 13:YB:459[B]:GLY:N | 13:YC:450[B]:VAL:O | 2.48 | 0.43 |
| 13:YB:476[C]:GLY:HA3 | 13:YC:469[C]:ASN:HA | 2.00 | 0.43 |
| 13:YC:76[D]:PRO:HG3 | 13:YC:96[D]:VAL:CG1 | 2.48 | 0.43 |
| 14:YD:233[C]:ASP:N | 14:YD:233[C]:ASP:OD1 | 2.51 | 0.43 |
| 14:YD:308[A]:ALA:O | 14:YD:357[A]:MET:N | 2.51 | 0.43 |
| 14:YD:308[D]:ALA:O | 14:YD:357[D]:MET:N | 2.52 | 0.43 |
| 14:YD:44[A]:LEU:HB2 | 14:YD:340[A]:ASP:O | 2.18 | 0.43 |
| 14:YD:80[A]:ILE:H | 14:YD:80[A]:ILE:HD13 | 1.83 | 0.43 |
| 14:YD:97[E]:VAL:HG12 | 14:YF:234[E]:PHE:HD1 | 1.83 | 0.43 |
| 13:YB:92[C]:THR:HB | 14:YE:282[C]:ALA:CB | 2.49 | 0.43 |
| 13:YB:92[F]:THR:HB | 14:YE:282[F]:ALA:CB | 2.48 | 0.43 |
| 14:YE:288[D]:TYR:CE1 | 14:YE:371[D]:LYS:HD3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:373[B]:LYS:HB3 | 14:YE:373[B]:LYS:HE2 | 1.86 | 0.43 |
| 14:YE:44[C]:LEU:HB2 | 14:YE:340[C]:ASP:O | 2.18 | 0.43 |
| 14:YE:80[E]:ILE:HD13 | 14:YE:80[E]:ILE:H | 1.83 | 0.43 |
| 14:YE:73[E]:SER:HA | 14:YE:85[E]:THR:HA | 2.01 | 0.43 |
| 10:BE:287:VAL:O | 14:YF:100[A]:LYS:HD3 | 2.18 | 0.43 |
| 14:YD:91[E]:LYS:O | 14:YF:242[E]:PRO:HD2 | 2.19 | 0.43 |
| 14:YF:308[D]:ALA:O | 14:YF:357[D]:MET:N | 2.51 | 0.43 |
| 14:YF:73[E]:SER:HA | 14:YF:85[E]:THR:HA | 2.00 | 0.43 |
| 2:Z:948:THR:HB | 2:Z:950:GLU:OE1 | 2.18 | 0.43 |
| 1:A:236:PHE:N | 1:A:236:PHE:CD1 | 2.84 | 0.43 |
| 5:AC:180:VAL:HG22 | 5:AC:181:PHE:H | 1.84 | 0.43 |
| 5:AD:253:GLN:HB2 | 5:AD:255:ARG:HE | 1.83 | 0.43 |
| 5:AD:68:TYR:HB2 | 5:AD:70:ILE:HD11 | 2.00 | 0.43 |
| 5:AC:407:TYR:CD1 | 5:AE:407:TYR:HB2 | 2.54 | 0.43 |
| 6:AG:86:ASP:CG | 6:AG:180:GLN:HE21 | 2.19 | 0.43 |
| 6:AH:88:TRP:O | 6:AH:155:LYS:HA | 2.18 | 0.43 |
| 7:AJ:198:GLN:HA | 7:AJ:201:GLN:CD | 2.38 | 0.43 |
| 7:AJ:232:THR:HG22 | 7:AJ:235:GLU:HG3 | 2.00 | 0.43 |
| 1:B:371:TYR:HB3 | 1:B:373:PHE:CE1 | 2.54 | 0.43 |
| 7:AI:39:ILE:HA | 7:BA:44:VAL:HG22 | 1.98 | 0.43 |
| 7:BA:2:SER:O | 7:BA:5:THR:HB | 2.18 | 0.43 |
| 8:BB:88:TRP:CE3 | 8:BB:134:PRO:HD3 | 2.53 | 0.43 |
| 8:BB:6:VAL:HB | 8:BC:53:PHE:CD1 | 2.53 | 0.43 |
| 11:BF:43:TYR:O | 11:BF:44:ARG:HB2 | 2.19 | 0.43 |
| 1:BH:113:THR:O | 1:BH:298:ILE:HG13 | 2.18 | 0.43 |
| 1:BI:188:TYR:HD1 | 1:BI:233:ASN:ND2 | 2.15 | 0.43 |
| 1:BI:330:THR:HG23 | 1:BI:333:ARG:HE | 1.83 | 0.43 |
| 1:BI:508:ARG:HE | 1:BI:544:ASP:HB2 | 1.83 | 0.43 |
| 1:BI:485:VAL:HG11 | 1:BI:650:TYR:CE1 | 2.53 | 0.43 |
| 2:BJ:251:ASP:CG | 2:BJ:252:LYS:HG3 | 2.38 | 0.43 |
| 2:BJ:404:TYR:CE1 | 2:BJ:415:ARG:HG2 | 2.53 | 0.43 |
| 2:BJ:420:THR:OG1 | 2:BJ:422:GLU:N | 2.51 | 0.43 |
| 2:BJ:455:VAL:CG2 | 2:BJ:472:LYS:HB3 | 2.49 | 0.43 |
| 2:C:108:TYR:CD2 | 2:C:108:TYR:N | 2.87 | 0.43 |
| 2:C:145:ALA:O | 2:C:586:LEU:HB3 | 2.18 | 0.43 |
| 2:C:146:LEU:HD12 | 2:C:146:LEU:C | 2.39 | 0.43 |
| 2:C:548:ILE:HG21 | 2:C:555:ARG:H | 1.84 | 0.43 |
| 2:C:135:VAL:HG12 | 2:C:589:LYS:HE3 | 2.00 | 0.43 |
| 3:CA:194:ILE:HG12 | 3:CA:223:TRP:HZ3 | 1.84 | 0.43 |
| 3:CA:72:TRP:CE2 | 3:CA:305:HIS:HA | 2.53 | 0.43 |
| 5:CF:222:LEU:HD11 | 5:CF:224:PRO:HD2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:258:TYR:CD2 | 5:CG:259:THR:N | 2.86 | 0.43 |
| 5:CF:317:LEU:HD13 | 5:CG:312:ARG:NH1 | 2.34 | 0.43 |
| 5:CH:293:PHE:HZ | 5:CH:366:PRO:O | 2.01 | 0.43 |
| 5:CG:569:TYR:HD1 | 5:CH:544:VAL:HA | 1.83 | 0.43 |
| 5:CH:478:TRP:CH2 | 5:CH:600:ARG:HB2 | 2.54 | 0.43 |
| 6:CJ:130:ARG:O | 6:CJ:134:GLN:HG3 | 2.18 | 0.43 |
| 6:CJ:47:PHE:HE2 | 6:CJ:51:ASN:HB3 | 1.84 | 0.43 |
| 6:DA:90:PHE:CD2 | 6:DA:126:VAL:HG22 | 2.45 | 0.43 |
| 6:DA:64:ILE:HG23 | 6:DA:217:ARG:HH12 | 1.84 | 0.43 |
| 7:DB:32:VAL:O | 7:DB:36:ILE:HG12 | 2.18 | 0.43 |
| 7:DC:342:PRO:HB2 | 7:DC:378:ARG:HH12 | 1.83 | 0.43 |
| 7:DD:182:THR:O | 7:DD:189:GLY:HA3 | 2.18 | 0.43 |
| 7:DD:21:THR:OG1 | 7:DD:22:ASP:N | 2.51 | 0.43 |
| 8:DE:15:PHE:N | 8:DE:15:PHE:CD1 | 2.84 | 0.43 |
| 9:DG:108:ILE:O | 9:DG:121:GLN:HA | 2.18 | 0.43 |
| 10:DH:237:THR:HA | 10:DH:287:VAL:CG2 | 2.47 | 0.43 |
| 10:DH:286:VAL:HG22 | 10:DH:287:VAL:N | 2.32 | 0.43 |
| 11:DI:186:ARG:HG3 | 11:DI:187:ILE:N | 2.33 | 0.43 |
| 1:EA:523:VAL:O | 1:EA:531:GLU:HB2 | 2.18 | 0.43 |
| 1:EA:595:ILE:HG21 | 1:EA:602:ILE:HG23 | 1.99 | 0.43 |
| 1:EB:122:TYR:HB3 | 1:EB:152:ILE:HD11 | 2.01 | 0.43 |
| 1:EB:205:GLU:C | 1:EB:206:TRP:HD1 | 2.21 | 0.43 |
| 2:EC:251:ASP:CG | 2:EC:252:LYS:HG3 | 2.38 | 0.43 |
| 2:EC:584:GLY:HA2 | 2:EC:600:PHE:CB | 2.46 | 0.43 |
| 4:EF:201:LYS:NZ | 4:EF:220:ASN:OD1 | 2.37 | 0.43 |
| 4:EG:168:PHE:CE1 | 4:EH:161:ASN:HB3 | 2.53 | 0.43 |
| 5:EI:477:SER:O | 5:EI:601:ILE:N | 2.50 | 0.43 |
| 5:EJ:190:ASN:HD22 | 5:EJ:247:PHE:HD2 | 1.65 | 0.43 |
| 5:EJ:341:GLU:C | 5:EJ:343:SER:H | 2.22 | 0.43 |
| 4:F:7:LYS:HD3 | 4:H:39:TYR:CD2 | 2.54 | 0.43 |
| 5:FA:71:ASN:ND2 | 5:FA:73:SER:OG | 2.52 | 0.43 |
| 6:FB:13:ARG:HG2 | 6:FB:14:LEU:N | 2.27 | 0.43 |
| 6:FD:13:ARG:HG2 | 6:FD:14:LEU:N | 2.27 | 0.43 |
| 7:FE:221:THR:HG23 | 7:FE:224:TYR:H | 1.83 | 0.43 |
| 7:FF:232:THR:HG22 | 7:FF:235:GLU:HG3 | 2.00 | 0.43 |
| 7:FF:451:PHE:HZ | 7:FF:471:THR:HG22 | 1.82 | 0.43 |
| 7:FF:77:THR:HG21 | 7:FG:72:ASN:CG | 2.39 | 0.43 |
| 7:FG:197:ALA:O | 7:FG:201:GLN:HG3 | 2.18 | 0.43 |
| 7:FG:2:SER:O | 7:FG:5:THR:HB | 2.18 | 0.43 |
| 7:FE:503:ASN:HD21 | 7:FG:446:LYS:H | 1.67 | 0.43 |
| 7:FE:76:VAL:N | 7:FG:76:VAL:O | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:557:PRO:HB3 | 1:GD:589:TYR:CZ | 2.53 | 0.43 |
| 1:GE:122:TYR:HB3 | 1:GE:152:ILE:HD11 | 2.01 | 0.43 |
| 2:GF:108:TYR:N | 2:GF:108:TYR:CD2 | 2.87 | 0.43 |
| 2:GF:404:TYR:CE1 | 2:GF:415:ARG:HG2 | 2.54 | 0.43 |
| 2:GF:420:THR:OG1 | 2:GF:422:GLU:N | 2.51 | 0.43 |
| 2:GF:548:ILE:HG21 | 2:GF:555:ARG:H | 1.84 | 0.43 |
| 3:GG:51:GLU:N | 3:GG:51:GLU:OE1 | 2.39 | 0.43 |
| 4:GI:69:LYS:NZ | 4:GJ:103:LEU:O | 2.32 | 0.43 |
| 4:GJ:192:PHE:CE1 | 4:GJ:197:TYR:HB2 | 2.53 | 0.43 |
| 4:GJ:28:GLY:O | 4:GJ:32:ASN:ND2 | 2.51 | 0.43 |
| 4:H:152:SER:O | 4:H:158:SER:HA | 2.18 | 0.43 |
| 4:HA:28:GLY:O | 4:HA:32:ASN:ND2 | 2.52 | 0.43 |
| 5:HB:180:VAL:HG22 | 5:HB:181:PHE:H | 1.83 | 0.43 |
| 5:HB:192:ARG:HG3 | 5:HB:245:GLU:HB2 | 1.99 | 0.43 |
| 5:HB:319:GLU:HG3 | 5:HC:262:GLN:OE1 | 2.19 | 0.43 |
| 5:HB:90:ASN:HD21 | 5:HC:49:TRP:C | 2.18 | 0.43 |
| 5:HD:357:SER:HA | 5:HD:371:PHE:CD1 | 2.54 | 0.43 |
| 6:HF:88:TRP:O | 6:HF:155:LYS:HA | 2.18 | 0.43 |
| 7:HH:167:GLN:O | 7:HH:171:LYS:HG2 | 2.18 | 0.43 |
| 7:HI:126:ASN:O | 7:HI:129:PHE:HB3 | 2.18 | 0.43 |
| 7:HJ:26:PRO:HA | 7:HJ:27:PRO:HD3 | 1.69 | 0.43 |
| 7:HJ:77:THR:HG22 | 7:HJ:80:THR:H | 1.82 | 0.43 |
| 5:I:180:VAL:HG22 | 5:I:181:PHE:H | 1.84 | 0.43 |
| 5:I:502:ASN:OD1 | 5:I:504:ASN:N | 2.52 | 0.43 |
| 11:IE:107:ASP:HA | 11:IE:155:THR:HG22 | 2.00 | 0.43 |
| 11:IE:166:LEU:HA | 11:IE:166:LEU:HD23 | 1.83 | 0.43 |
| 11:IE:44:ARG:HG2 | 11:IE:45:LEU:N | 2.33 | 0.43 |
| 5:J:253:GLN:HB2 | 5:J:255:ARG:HE | 1.83 | 0.43 |
| 5:I:319:GLU:HG3 | 5:J:262:GLN:OE1 | 2.18 | 0.43 |
| 5:K:357:SER:HA | 5:K:371:PHE:CD1 | 2.54 | 0.43 |
| 5:I:549:SER:N | 5:K:569:TYR:O | 2.51 | 0.43 |
| 7:P:201:GLN:HG2 | 6:HG:27:ILE:HG21 | 1.99 | 0.43 |
| 5:K:196:ARG:HH11 | 7:P:8:HIS:HB3 | 1.83 | 0.43 |
| 7:O:95:TYR:HD1 | 7:Q:99:ARG:N | 2.17 | 0.43 |
| 8:S:150:ILE:HD11 | 8:IB:15:PHE:CB | 2.48 | 0.43 |
| 9:T:10:ASP:OD1 | 9:T:11:ILE:HG22 | 2.18 | 0.43 |
| 12:W:8:ASN:HA | 12:W:12:ILE:HG22 | 2.00 | 0.43 |
| 1:X:157:LYS:O | 1:X:158:ASN:CG | 2.57 | 0.43 |
| 1:X:90:VAL:HG11 | 1:X:228:GLU:HG2 | 2.01 | 0.43 |
| 1:X:365:ASP:OD2 | 1:X:367:THR:HB | 2.18 | 0.43 |
| 1:Y:205:GLU:C | 1:Y:206:TRP:HD1 | 2.21 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:559:ALA:HB3 | 1:Y:562:ASP:OD2 | 2.18 | 0.43 |
| 13:YA:109[C]:ASN:OD1 | 13:YA:110[C]:ARG:N | 2.51 | 0.43 |
| 13:YA:109[E]:ASN:OD1 | 13:YA:110[E]:ARG:N | 2.51 | 0.43 |
| 13:YA:200[E]:ILE:HD13 | 13:YA:236[E]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:209[E]:GLN:HB2 | 13:YA:209[E]:GLN:HE21 | 1.64 | 0.43 |
| 13:YA:280[E]:MET:O | 13:YA:284[E]:MET:HG2 | 2.19 | 0.43 |
| 13:YA:280[B]:MET:O | 13:YA:284[B]:MET:HG2 | 2.19 | 0.43 |
| 13:YA:363[A]:PRO:HB2 | 13:YC:284[A]:MET:HE3 | 2.01 | 0.43 |
| 13:YA:363[D]:PRO:HB2 | 13:YC:284[D]:MET:HE3 | 2.01 | 0.43 |
| 13:YA:389[C]:TYR:O | 13:YA:405[C]:ASP:HB2 | 2.18 | 0.43 |
| 13:YA:47[B]:ILE:HG12 | 14:YD:123[B]:PRO:HD3 | 1.99 | 0.43 |
| 13:YA:534[E]:LEU:HD11 | 13:YA:536[E]:TRP:NE1 | 2.32 | 0.43 |
| 13:YA:59[B]:GLN:HA | 13:YC:61[B]:ILE:CG2 | 2.49 | 0.43 |
| 13:YB:127[C]:ASN:ND2 | 13:YB:129[C]:THR:OG1 | 2.52 | 0.43 |
| 13:YB:187[E]:ARG:HD3 | 13:YB:187[E]:ARG:HA | 1.87 | 0.43 |
| 13:YB:200[E]:ILE:HD13 | 13:YB:236[E]:ILE:HD12 | 2.01 | 0.43 |
| 13:YB:252[D]:MET:HE3 | 13:YB:252[D]:MET:HB3 | 1.87 | 0.43 |
| 13:YB:263[C]:GLY:N | 13:YB:264[C]:PRO:HD2 | 2.33 | 0.43 |
| 13:YB:257[D]:LYS:HE2 | 13:YB:266[D]:TRP:CH2 | 2.53 | 0.43 |
| 13:YB:280[B]:MET:O | 13:YB:284[B]:MET:HG2 | 2.19 | 0.43 |
| 13:YB:442[A]:THR:HB | 13:YC:434[A]:THR:HB | 2.00 | 0.43 |
| 13:YA:471[A]:LEU:O | 13:YB:463[A]:ILE:HA | 2.18 | 0.43 |
| 13:YB:50[A]:GLU:N | 13:YB:50[A]:GLU:CD | 2.71 | 0.43 |
| 13:YA:551[D]:THR:O | 13:YB:543[D]:ASP:HA | 2.19 | 0.43 |
| 13:YA:551[E]:THR:O | 13:YB:543[E]:ASP:HA | 2.19 | 0.43 |
| 13:YA:569[E]:GLY:HA2 | 13:YB:561[E]:SER:O | 2.19 | 0.43 |
| 13:YB:564[B]:GLN:HG3 | 13:YB:566[B]:THR:HG22 | 2.01 | 0.43 |
| 13:YC:112[F]:GLU:C | 13:YC:115[F]:SER:HB3 | 2.39 | 0.43 |
| 13:YB:73[C]:VAL:HG21 | 13:YC:129[C]:THR:HG22 | 2.01 | 0.43 |
| 13:YC:36[D]:PRO:HB2 | 13:YC:38[D]:GLN:OE1 | 2.17 | 0.43 |
| 13:YB:458[F]:VAL:HG21 | 13:YC:454[F]:LYS:HD2 | 2.00 | 0.43 |
| 13:YA:534[D]:LEU:CB | 13:YC:538[D]:VAL:HG11 | 2.47 | 0.43 |
| 13:YA:9[D]:ASN:ND2 | 13:YC:7[D]:ASN:OD1 | 2.51 | 0.43 |
| 13:YC:83[B]:TYR:OH | 13:YC:85[B]:HIS:HE1 | 2.02 | 0.43 |
| 14:YD:101[A]:GLY:HA3 | 14:YF:330[A]:LYS:HG2 | 2.01 | 0.43 |
| 14:YD:109[E]:LEU:HD12 | 14:YD:109[E]:LEU:HA | 1.65 | 0.43 |
| 14:YD:127[D]:ASP:CG | 14:YD:130[D]:GLU:H | 2.19 | 0.43 |
| 14:YD:234[F]:PHE:HD1 | 14:YE:97[F]:VAL:HG12 | 1.84 | 0.43 |
| 14:YD:80[B]:ILE:HD13 | 14:YD:80[B]:ILE:H | 1.83 | 0.43 |
| 14:YD:330[D]:LYS:HG2 | 14:YE:101[D]:GLY:HA3 | 2.00 | 0.43 |
| 14:YE:109[C]:LEU:HD12 | 14:YE:109[C]:LEU:HA | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:132[B]:ILE:HD12 | 14:YE:197[B]:MET:SD | 2.58 | 0.43 |
| 14:YE:132[E]:ILE:HD12 | 14:YE:197[E]:MET:SD | 2.58 | 0.43 |
| 14:YE:132[D]:ILE:HD12 | 14:YE:197[D]:MET:SD | 2.58 | 0.43 |
| 14:YE:308[C]:ALA:O | 14:YE:357[C]:MET:N | 2.52 | 0.43 |
| 14:YE:308[D]:ALA:O | 14:YE:357[D]:MET:N | 2.52 | 0.43 |
| 14:YE:80[D]:ILE:HD13 | 14:YE:80[D]:ILE:H | 1.83 | 0.43 |
| 14:YE:88[C]:TYR:HD1 | 14:YE:110[C]:GLY:C | 2.21 | 0.43 |
| 14:YF:132[F]:ILE:HD12 | 14:YF:197[F]:MET:SD | 2.58 | 0.43 |
| 14:YF:277[B]:VAL:HG11 | 14:YF:294[B]:GLU:HG2 | 1.99 | 0.43 |
| 2:Z:160:VAL:O | 2:Z:163:ILE:HB | 2.18 | 0.43 |
| 2:Z:404:TYR:CE1 | 2:Z:415:ARG:HG2 | 2.54 | 0.43 |
| 2:Z:135:VAL:HG12 | 2:Z:589:LYS:HE3 | 2.01 | 0.43 |
| 15:ZA:26[B]:GLN:NE2 | 15:ZA:29[B]:VAL:H | 1.93 | 0.43 |
| 1:A:336:GLN:HG3 | 1:A:337:GLN:N | 2.31 | 0.43 |
| 1:A:38:ASN:N | 1:A:48:PHE:HE2 | 2.17 | 0.43 |
| 1:A:79:PHE:CE1 | 2:C:702:GLU:HG2 | 2.52 | 0.43 |
| 4:AA:28:GLY:O | 4:AA:32:ASN:ND2 | 2.51 | 0.43 |
| 4:AA:61:ILE:HB | 4:AB:4:GLN:OE1 | 2.19 | 0.43 |
| 5:AC:150:GLN:HG3 | 5:AC:151:ILE:O | 2.18 | 0.43 |
| 5:AC:181:PHE:HE2 | 5:AC:246:THR:HG22 | 1.83 | 0.43 |
| 5:AC:222:LEU:HD11 | 5:AC:224:PRO:HD2 | 2.01 | 0.43 |
| 5:AC:320:LEU:HG | 5:AC:357:SER:CB | 2.49 | 0.43 |
| 5:AD:258:TYR:CD2 | 5:AD:259:THR:N | 2.86 | 0.43 |
| 5:AD:363:ASN:N | 5:AD:367:GLU:OE2 | 2.49 | 0.43 |
| 6:AF:108:LEU:HD23 | 6:AF:113:PRO:HA | 2.00 | 0.43 |
| 6:AH:64:ILE:HG23 | 6:AH:217:ARG:HH12 | 1.84 | 0.43 |
| 7:AI:87:TYR:HA | 7:DB:412:PRO:CG | 2.49 | 0.43 |
| 7:AI:141:VAL:HG23 | 7:AJ:140:GLY:O | 2.19 | 0.43 |
| 7:AI:509:GLY:O | 7:AJ:443:SER:HA | 2.18 | 0.43 |
| 7:AJ:66:VAL:HG21 | 7:AJ:80:THR:HB | 2.01 | 0.43 |
| 1:B:559:ALA:HB3 | 1:B:562:ASP:OD2 | 2.18 | 0.43 |
| 7:BA:413:ASN:O | 7:BA:424:ARG:HD3 | 2.17 | 0.43 |
| 7:AI:408:HIS:CE1 | 7:BA:437:VAL:HG21 | 2.53 | 0.43 |
| 9:BD:10:ASP:OD1 | 9:BD:11:ILE:HG22 | 2.18 | 0.43 |
| 9:BD:108:ILE:O | 9:BD:121:GLN:HA | 2.18 | 0.43 |
| 1:BH:485:VAL:HG22 | 1:BH:624:TYR:CD1 | 2.53 | 0.43 |
| 1:BH:38:ASN:N | 1:BH:48:PHE:HE2 | 2.17 | 0.43 |
| 1:BH:561:GLY:H | 1:BH:588:LYS:NZ | 2.16 | 0.43 |
| 1:BI:373:PHE:O | 1:BI:374:ILE:HD13 | 2.18 | 0.43 |
| 1:BI:485:VAL:HG22 | 1:BI:624:TYR:HD1 | 1.83 | 0.43 |
| 2:BJ:450:PHE:HE2 | 2:BJ:473:TYR:HH | 1.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BJ:725:ARG:HA | 2:BJ:728:GLU:HB3 | 2.00 | 0.43 |
| 2:C:194:GLU:HG2 | 2:C:199:LEU:HA | 2.01 | 0.43 |
| 2:C:927:THR:HB | 2:C:987:ARG:HA | 2.00 | 0.43 |
| 2:C:9:THR:OG1 | 2:C:10:SER:N | 2.51 | 0.43 |
| 4:CE:28:GLY:O | 4:CE:32:ASN:ND2 | 2.52 | 0.43 |
| 5:CF:196:ARG:O | 5:CH:197:GLY:HA2 | 2.19 | 0.43 |
| 5:CF:275:SER:OG | 5:CF:281:TYR:HA | 2.19 | 0.43 |
| 5:CF:424:ASP:OD2 | 5:CF:427:LYS:HB3 | 2.19 | 0.43 |
| 5:CG:267:ASP:H | 5:CG:377:HIS:HB2 | 1.84 | 0.43 |
| 5:CH:102:TRP:CZ3 | 5:CH:131:SER:HB2 | 2.53 | 0.43 |
| 3:D:150:LYS:HE2 | 3:D:160:TRP:CD1 | 2.53 | 0.43 |
| 3:D:71:MET:HE1 | 3:D:271:GLN:HG2 | 1.99 | 0.43 |
| 7:DB:221:THR:HG23 | 7:DB:224:TYR:H | 1.83 | 0.43 |
| 7:DC:354:LEU:HD21 | 7:DC:522:ILE:HG21 | 2.00 | 0.43 |
| 7:DC:375:TYR:CZ | 7:DC:392:LEU:HD23 | 2.53 | 0.43 |
| 11:DI:36:PHE:HZ | 11:DI:76:CYS:SG | 2.40 | 0.43 |
| 12:DJ:22:PHE:CG | 12:GC:228:LEU:HD13 | 2.53 | 0.43 |
| 3:E:135:ASP:H | 3:E:187:VAL:HG12 | 1.82 | 0.43 |
| 1:EA:123:ILE:HD12 | 1:EA:123:ILE:HA | 1.76 | 0.43 |
| 1:EB:377:LYS:HB3 | 1:EB:377:LYS:HE2 | 1.65 | 0.43 |
| 3:CB:265:GLY:HA3 | 1:EB:656:GLU:OE2 | 2.19 | 0.43 |
| 2:EC:114:ILE:HG23 | 2:EC:115:GLU:N | 2.33 | 0.43 |
| 2:EC:376:PHE:CZ | 2:EC:441:VAL:HG11 | 2.51 | 0.43 |
| 4:EF:28:GLY:O | 4:EF:32:ASN:ND2 | 2.51 | 0.43 |
| 4:EG:190:PRO:HA | 4:EG:262:THR:HA | 2.01 | 0.43 |
| 4:EH:209:VAL:HG13 | 4:EH:271:GLY:O | 2.19 | 0.43 |
| 4:EG:39:TYR:CG | 4:EH:7:LYS:HD3 | 2.53 | 0.43 |
| 5:EI:290:SER:HA | 5:EI:371:PHE:H | 1.82 | 0.43 |
| 5:EJ:71:ASN:HB2 | 5:EJ:99:PHE:HZ | 1.82 | 0.43 |
| 4:F:28:GLY:O | 4:F:32:ASN:ND2 | 2.51 | 0.43 |
| 5:FA:130:PHE:HD2 | 5:FA:152:ASP:HB2 | 1.83 | 0.43 |
| 5:EJ:483:GLN:NE2 | 5:FA:492:GLU:HG2 | 2.33 | 0.43 |
| 5:FA:49:TRP:CZ3 | 5:FA:96:ARG:HD2 | 2.54 | 0.43 |
| 6:FB:13:ARG:NH1 | 6:FD:47:PHE:CE1 | 2.87 | 0.43 |
| 6:FB:73:ASN:HB3 | 6:FD:69:THR:HA | 2.00 | 0.43 |
| 6:FD:201:VAL:N | 6:FD:210:THR:O | 2.31 | 0.43 |
| 7:FE:192:GLN:HG3 | 7:FF:188:GLN:CD | 2.39 | 0.43 |
| 7:FE:77:THR:HG22 | 7:FE:80:THR:H | 1.83 | 0.43 |
| 7:FE:97:LEU:HD23 | 7:FG:97:LEU:CD2 | 2.48 | 0.43 |
| 7:FF:227:VAL:HG23 | 7:FG:225:LYS:HB3 | 1.99 | 0.43 |
| 7:FE:425:LEU:HD11 | 7:FF:505:PRO:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FH:3:VAL:HG21 | 8:FI:56:ARG:NH2 | 2.34 | 0.43 |
| 10:GA:237:THR:HA | 10:GA:287:VAL:CG2 | 2.47 | 0.43 |
| 12:DJ:153:ARG:NH2 | 12:GC:184:PRO:HA | 2.33 | 0.43 |
| 12:GC:8:ASN:HA | 12:GC:12:ILE:HG22 | 2.00 | 0.43 |
| 2:GF:186:ASP:HB3 | 2:GF:189:ARG:CD | 2.49 | 0.43 |
| 2:GF:506:MET:HB3 | 2:GF:506:MET:HE2 | 1.94 | 0.43 |
| 2:GF:669:GLU:O | 2:GF:672:ILE:N | 2.51 | 0.43 |
| 3:GH:140:GLY:HA2 | 3:GH:163:SER:N | 2.33 | 0.43 |
| 4:GJ:168:PHE:CE1 | 4:HA:161:ASN:HB3 | 2.54 | 0.43 |
| 5:HC:258:TYR:CD2 | 5:HC:259:THR:N | 2.87 | 0.43 |
| 5:HC:275:SER:OG | 5:HC:281:TYR:HA | 2.19 | 0.43 |
| 5:HC:395:THR:OG1 | 5:HC:396:LYS:N | 2.52 | 0.43 |
| 5:HC:71:ASN:HB2 | 5:HC:99:PHE:HZ | 1.82 | 0.43 |
| 5:HD:131:SER:HA | 5:HD:150:GLN:HA | 1.99 | 0.43 |
| 5:HD:352:SER:HB2 | 5:HD:354:THR:O | 2.18 | 0.43 |
| 5:HD:49:TRP:CZ3 | 5:HD:96:ARG:HD2 | 2.54 | 0.43 |
| 6:HE:130:ARG:O | 6:HE:134:GLN:HG3 | 2.18 | 0.43 |
| 6:HE:47:PHE:HE2 | 6:HE:51:ASN:HB3 | 1.84 | 0.43 |
| 6:HF:108:LEU:HD23 | 6:HF:113:PRO:HA | 2.00 | 0.43 |
| 6:HF:90:PHE:O | 6:HF:154:SER:HB2 | 2.19 | 0.43 |
| 7:HH:102:THR:O | 7:HH:105:GLU:N | 2.52 | 0.43 |
| 7:HH:262:VAL:HB | 7:HI:261:GLY:N | 2.32 | 0.43 |
| 7:HH:425:LEU:HD11 | 7:HI:505:PRO:O | 2.19 | 0.43 |
| 7:HH:475:LEU:HA | 7:HI:470:GLY:O | 2.18 | 0.43 |
| 7:HI:117:THR:HB | 7:HJ:112:ASN:HA | 1.99 | 0.43 |
| 7:HI:31:ASP:CG | 7:HI:34:ALA:H | 2.18 | 0.43 |
| 7:HH:299:THR:O | 7:HJ:293:GLY:N | 2.50 | 0.43 |
| 7:HI:477:TRP:CZ3 | 7:HJ:469:VAL:HB | 2.53 | 0.43 |
| 7:HH:472:ARG:NH1 | 7:HJ:474:GLY:HA2 | 2.34 | 0.43 |
| 5:I:262:GLN:HA | 5:I:381:ILE:O | 2.17 | 0.43 |
| 5:I:293:PHE:HA | 5:I:295:ALA:H | 1.82 | 0.43 |
| 5:I:522:SER:C | 5:K:591:PRO:HD3 | 2.38 | 0.43 |
| 10:ID:237:THR:HA | 10:ID:287:VAL:CG2 | 2.47 | 0.43 |
| 11:IE:31:ASN:O | 11:IE:32:TYR:HB2 | 2.18 | 0.43 |
| 12:IF:164:MET:HB3 | 12:IF:237:THR:HG22 | 2.01 | 0.43 |
| 5:K:89:TYR:CE1 | 5:K:139:ALA:HA | 2.54 | 0.43 |
| 5:K:478:TRP:CH2 | 5:K:600:ARG:HB2 | 2.54 | 0.43 |
| 5:J:597:ARG:HH12 | 5:K:489:GLY:N | 2.16 | 0.43 |
| 6:M:108:LEU:HD23 | 6:M:113:PRO:HA | 2.00 | 0.43 |
| 6:M:47:PHE:HE2 | 6:M:51:ASN:HB3 | 1.84 | 0.43 |
| 7:O:299:THR:O | 7:Q:293:GLY:N | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:509:GLY:O | 7:P:443:SER:HA | 2.19 | 0.43 |
| 7:O:162:PRO:CB | 7:P:150:ALA:HA | 2.48 | 0.43 |
| 7:P:354:LEU:HD21 | 7:P:522:ILE:HG21 | 2.00 | 0.43 |
| 5:J:200:LEU:HB2 | 7:P:5:THR:HG21 | 1.99 | 0.43 |
| 7:P:77:THR:CG2 | 7:P:80:THR:H | 2.31 | 0.43 |
| 7:Q:134:SER:HB3 | 7:Q:140:GLY:N | 2.33 | 0.43 |
| 7:Q:21:THR:OG1 | 7:Q:22:ASP:N | 2.51 | 0.43 |
| 7:P:227:VAL:CG2 | 7:Q:225:LYS:HB3 | 2.49 | 0.43 |
| 8:S:150:ILE:HD11 | 8:IB:15:PHE:HB2 | 2.00 | 0.43 |
| 11:V:186:ARG:HG3 | 11:V:187:ILE:N | 2.33 | 0.43 |
| 11:V:88:THR:HG22 | 11:V:92:ALA:HB3 | 1.99 | 0.43 |
| 1:X:341:THR:HG23 | 2:Z:880:ILE:O | 2.19 | 0.43 |
| 1:X:413:TYR:CE1 | 1:X:415:PHE:HE1 | 2.36 | 0.43 |
| 1:X:557:PRO:HB3 | 1:X:589:TYR:CZ | 2.53 | 0.43 |
| 1:X:561:GLY:H | 1:X:588:LYS:NZ | 2.16 | 0.43 |
| 1:X:508:ARG:HH22 | 1:X:577:PHE:HA | 1.84 | 0.43 |
| 1:X:619:GLN:CD | 1:X:619:GLN:H | 2.18 | 0.43 |
| 13:YA:112[D]:GLU:C | 13:YA:115[D]:SER:HB3 | 2.39 | 0.43 |
| 13:YA:127[E]:ASN:ND2 | 13:YA:129[E]:THR:OG1 | 2.52 | 0.43 |
| 13:YA:132[B]:LEU:O | 13:YA:390[B]:VAL:HG11 | 2.19 | 0.43 |
| 13:YA:147[D]:ILE:HD11 | 13:YA:188[D]:LEU:HG | 2.00 | 0.43 |
| 13:YA:327[E]:VAL:O | 13:YA:331[E]:ILE:HG22 | 2.19 | 0.43 |
| 13:YA:327[B]:VAL:O | 13:YA:331[B]:ILE:HG22 | 2.19 | 0.43 |
| 13:YA:363[E]:PRO:HB2 | 13:YC:284[E]:MET:HE3 | 2.00 | 0.43 |
| 13:YA:36[A]:PRO:HB2 | 13:YA:38[A]:GLN:OE1 | 2.17 | 0.43 |
| 13:YA:394[C]:GLU:N | 13:YC:70[C]:GLY:O | 2.50 | 0.43 |
| 13:YA:473[B]:GLN:OE1 | 13:YC:158[B]:PRO:HB2 | 2.18 | 0.43 |
| 13:YA:552[A]:GLU:CG | 13:YA:554[A]:MET:HE1 | 2.49 | 0.43 |
| 13:YB:200[F]:ILE:HD13 | 13:YB:236[F]:ILE:HD12 | 2.01 | 0.43 |
| 13:YB:263[E]:GLY:N | 13:YB:264[E]:PRO:HD2 | 2.33 | 0.43 |
| 13:YB:278[B]:GLU:O | 13:YB:282[B]:PHE:N | 2.51 | 0.43 |
| 13:YB:278[F]:GLU:O | 13:YB:282[F]:PHE:N | 2.52 | 0.43 |
| 13:YB:320[E]:THR:HG22 | 13:YB:323[E]:ARG:HB3 | 2.00 | 0.43 |
| 13:YB:330[C]:ILE:HD12 | 13:YB:336[C]:LEU:HD12 | 2.00 | 0.43 |
| 13:YB:389[D]:TYR:O | 13:YB:405[D]:ASP:HB2 | 2.19 | 0.43 |
| 13:YB:458[A]:VAL:HG21 | 13:YC:454[A]:LYS:HD2 | 1.99 | 0.43 |
| 13:YA:558[F]:SER:N | 13:YB:550[F]:TRP:O | 2.50 | 0.43 |
| 13:YC:112[A]:GLU:C | 13:YC:115[A]:SER:HB3 | 2.39 | 0.43 |
| 13:YC:112[D]:GLU:C | 13:YC:115[D]:SER:HB3 | 2.39 | 0.43 |
| 13:YC:147[F]:ILE:HD11 | 13:YC:188[F]:LEU:HG | 2.00 | 0.43 |
| 13:YC:147[E]:ILE:HD11 | 13:YC:188[E]:LEU:HG | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:219[F]:LYS:HB2 | 13:YC:219[F]:LYS:HE3 | 1.81 | 0.43 |
| 13:YC:257[A]:LYS:HE2 | 13:YC:266[A]:TRP:CH2 | 2.53 | 0.43 |
| 13:YC:320[C]:THR:HG22 | 13:YC:323[C]:ARG:HB3 | 2.00 | 0.43 |
| 13:YC:36[C]:PRO:HB2 | 13:YC:38[C]:GLN:OE1 | 2.17 | 0.43 |
| 13:YC:389[A]:TYR:O | 13:YC:405[A]:ASP:HB2 | 2.19 | 0.43 |
| 13:YC:389[C]:TYR:O | 13:YC:405[C]:ASP:HB2 | 2.18 | 0.43 |
| 13:YB:530[C]:VAL:HG22 | 13:YC:522[C]:VAL:HG13 | 2.01 | 0.43 |
| 13:YA:544[E]:TRP:HB2 | 13:YC:552[E]:GLU:HB2 | 2.00 | 0.43 |
| 13:YC:552[C]:GLU:CG | 13:YC:554[C]:MET:HE1 | 2.49 | 0.43 |
| 13:YC:564[F]:GLN:HG3 | 13:YC:566[F]:THR:HG22 | 2.01 | 0.43 |
| 13:YA:9[C]:ASN:ND2 | 13:YC:7[C]:ASN:OD1 | 2.51 | 0.43 |
| 14:YD:233[D]:ASP:OD1 | 14:YD:233[D]:ASP:N | 2.51 | 0.43 |
| 14:YD:277[E]:VAL:HG11 | 14:YD:294[E]:GLU:HG2 | 1.98 | 0.43 |
| 14:YD:44[E]:LEU:HB2 | 14:YD:340[E]:ASP:O | 2.18 | 0.43 |
| 14:YD:80[F]:ILE:HD13 | 14:YD:80[F]:ILE:H | 1.83 | 0.43 |
| 13:YB:26[E]:ARG:HD3 | 14:YE:259[E]:LEU:CD2 | 2.48 | 0.43 |
| 14:YE:277[B]:VAL:HG11 | 14:YE:294[B]:GLU:HG2 | 1.99 | 0.43 |
| 14:YE:308[A]:ALA:O | 14:YE:357[A]:MET:N | 2.51 | 0.43 |
| 14:YE:80[F]:ILE:H | 14:YE:80[F]:ILE:HD13 | 1.83 | 0.43 |
| 14:YF:132[B]:ILE:HD12 | 14:YF:197[B]:MET:SD | 2.58 | 0.43 |
| 14:YD:101[D]:GLY:HA3 | 14:YF:330[D]:LYS:HG2 | 2.00 | 0.43 |
| 14:YF:373[F]:LYS:HB3 | 14:YF:373[F]:LYS:HE2 | 1.87 | 0.43 |
| 14:YF:80[D]:ILE:HD13 | 14:YF:80[D]:ILE:H | 1.83 | 0.43 |
| 2:Z:168:ILE:CG2 | 2:Z:169:GLY:N | 2.81 | 0.43 |
| 2:Z:186:ASP:HB3 | 2:Z:189:ARG:CD | 2.49 | 0.43 |
| 2:Z:420:THR:OG1 | 2:Z:422:GLU:N | 2.51 | 0.43 |
| 2:Z:455:VAL:CG2 | 2:Z:472:LYS:HB3 | 2.49 | 0.43 |
| 2:Z:613:LYS:HG3 | 2:Z:614:PRO:HD3 | 2.00 | 0.43 |
| 15:ZA:37[B]:LEU:HB2 | 15:ZA:75[B]:VAL:HB | 2.01 | 0.43 |
| 15:ZA:37[C]:LEU:HB2 | 15:ZA:75[C]:VAL:HB | 2.01 | 0.43 |
| 4:AB:28:GLY:O | 4:AB:32:ASN:ND2 | 2.51 | 0.43 |
| 5:AC:139:ALA:O | 5:AC:141:GLY:N | 2.47 | 0.43 |
| 5:AC:358:VAL:HG23 | 5:AC:371:PHE:HD1 | 1.83 | 0.43 |
| 5:AC:469:PRO:HA | 5:AC:472:TYR:CZ | 2.54 | 0.43 |
| 5:AC:64:TRP:CZ2 | 5:AC:82:PRO:HB2 | 2.54 | 0.43 |
| 6:AF:47:PHE:HE2 | 6:AF:51:ASN:HB3 | 1.84 | 0.43 |
| 6:AG:90:PHE:CD2 | 6:AG:126:VAL:HG22 | 2.45 | 0.43 |
| 6:AG:47:PHE:HE2 | 6:AG:51:ASN:HB3 | 1.84 | 0.43 |
| 6:AH:90:PHE:O | 6:AH:154:SER:HB2 | 2.19 | 0.43 |
| 5:AC:318:GLN:NE2 | 6:AH:4:LEU:O | 2.50 | 0.43 |
| 7:AI:444:TYR:HB2 | 7:BA:486:ASP:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:533:ASP:OD1 | 1:B:534:VAL:HG22 | 2.18 | 0.43 |
| 1:A:67:ILE:HD11 | 1:B:67:ILE:HG21 | 2.00 | 0.43 |
| 1:B:90:VAL:O | 1:B:94:GLN:HG2 | 2.17 | 0.43 |
| 7:BA:134:SER:HB3 | 7:BA:140:GLY:N | 2.33 | 0.43 |
| 7:AI:188:GLN:NE2 | 7:BA:192:GLN:OE1 | 2.52 | 0.43 |
| 7:BA:20:PRO:CD | 7:BA:29:ILE:HG21 | 2.49 | 0.43 |
| 7:BA:489:GLU:CD | 7:BA:502:LEU:H | 2.22 | 0.43 |
| 8:BB:22:GLN:OE1 | 8:BB:116:TYR:OH | 2.25 | 0.43 |
| 11:BF:44:ARG:HG2 | 11:BF:45:LEU:N | 2.33 | 0.43 |
| 1:BH:123:ILE:HD11 | 1:BH:295:ILE:HD11 | 2.00 | 0.43 |
| 1:BH:525:ASN:HB3 | 1:BH:528:THR:CG2 | 2.48 | 0.43 |
| 1:BI:276:ASN:HB2 | 1:BI:279:ASP:OD2 | 2.18 | 0.43 |
| 2:BJ:1005:ARG:HG2 | 2:BJ:1006:ASP:O | 2.19 | 0.43 |
| 2:BJ:151:PHE:HB3 | 2:BJ:166:PHE:HZ | 1.83 | 0.43 |
| 2:BJ:52:ASN:O | 2:BJ:54:TYR:N | 2.51 | 0.43 |
| 2:BJ:798:ILE:HG12 | 2:BJ:811:VAL:HG12 | 2.00 | 0.43 |
| 2:BJ:897:THR:O | 2:BJ:898:MET:HE2 | 2.18 | 0.43 |
| 2:C:213:ASN:HB2 | 2:C:289:PHE:CZ | 2.53 | 0.43 |
| 2:C:669:GLU:O | 2:C:672:ILE:N | 2.52 | 0.43 |
| 2:C:948:THR:HB | 2:C:950:GLU:OE1 | 2.18 | 0.43 |
| 3:CB:140:GLY:HA2 | 3:CB:163:SER:N | 2.33 | 0.43 |
| 3:CB:71:MET:SD | 3:CB:312:MET:HG2 | 2.58 | 0.43 |
| 4:CD:190:PRO:HA | 4:CD:262:THR:HA | 2.01 | 0.43 |
| 5:CF:184:THR:H | 5:CF:307:ASN:ND2 | 2.13 | 0.43 |
| 5:CG:104:VAL:HG22 | 5:CG:105:ASN:H | 1.83 | 0.43 |
| 5:CH:133:LEU:HD23 | 5:CH:133:LEU:HA | 1.81 | 0.43 |
| 5:CH:338:ASP:HB3 | 5:CH:349:TRP:HD1 | 1.78 | 0.43 |
| 5:CH:352:SER:HB2 | 5:CH:354:THR:O | 2.18 | 0.43 |
| 2:BJ:228:ARG:NH2 | 5:CH:559:PRO:HB3 | 2.28 | 0.43 |
| 6:CI:87:TYR:N | 6:CI:181:GLU:O | 2.32 | 0.43 |
| 3:D:131:TYR:HD1 | 3:D:190:TYR:HA | 1.84 | 0.43 |
| 7:DB:167:GLN:O | 7:DB:171:LYS:HG2 | 2.18 | 0.43 |
| 7:DB:176:ILE:HG23 | 7:DB:177:ALA:H | 1.84 | 0.43 |
| 7:DC:66:VAL:HG21 | 7:DC:80:THR:HB | 2.01 | 0.43 |
| 7:DD:125:LEU:O | 7:DD:129:PHE:N | 2.40 | 0.43 |
| 7:DD:161:THR:H | 7:DD:164:LYS:HB2 | 1.83 | 0.43 |
| 7:DD:218:SER:O | 7:DD:227:VAL:HG22 | 2.19 | 0.43 |
| 5:CG:196:ARG:HH22 | 7:DD:9:VAL:HG12 | 1.83 | 0.43 |
| 9:DG:47:ARG:HA | 9:DG:47:ARG:HD2 | 1.79 | 0.43 |
| 12:DJ:140:ASP:OD1 | 12:DJ:141:TRP:N | 2.52 | 0.43 |
| 3:E:228:ASN:HA | 3:E:229:LEU:HD13 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:401:LEU:HA | 1:EB:401:LEU:HD23 | 1.87 | 0.43 |
| 2:EC:114:ILE:HG23 | 2:EC:115:GLU:H | 1.83 | 0.43 |
| 2:EC:160:VAL:O | 2:EC:163:ILE:HB | 2.18 | 0.43 |
| 2:EC:194:GLU:HG2 | 2:EC:199:LEU:HA | 2.01 | 0.43 |
| 2:EC:404:TYR:CE1 | 2:EC:415:ARG:HG2 | 2.54 | 0.43 |
| 2:EC:450:PHE:HE2 | 2:EC:473:TYR:HH | 1.65 | 0.43 |
| 1:EA:64:THR:HG21 | 2:EC:674:TYR:HE2 | 1.83 | 0.43 |
| 2:EC:706:SER:O | 2:EC:708:ILE:N | 2.42 | 0.43 |
| 2:EC:798:ILE:HG12 | 2:EC:811:VAL:HG12 | 2.00 | 0.43 |
| 2:EC:883:VAL:HG13 | 2:EC:884:HIS:H | 1.82 | 0.43 |
| 3:ED:131:TYR:HD1 | 3:ED:190:TYR:HA | 1.84 | 0.43 |
| 4:EF:209:VAL:HG13 | 4:EF:271:GLY:O | 2.19 | 0.43 |
| 5:EI:181:PHE:HE2 | 5:EI:246:THR:HG22 | 1.83 | 0.43 |
| 5:EI:502:ASN:OD1 | 5:EI:504:ASN:N | 2.51 | 0.43 |
| 5:EJ:253:GLN:HB2 | 5:EJ:255:ARG:HE | 1.84 | 0.43 |
| 5:EJ:68:TYR:HB2 | 5:EJ:70:ILE:HD11 | 2.00 | 0.43 |
| 4:F:201:LYS:NZ | 4:F:220:ASN:OD1 | 2.37 | 0.43 |
| 5:FA:158:ASP:OD1 | 5:FA:159:ILE:N | 2.47 | 0.43 |
| 5:FA:177:PHE:CD2 | 5:FA:230:ILE:HD11 | 2.48 | 0.43 |
| 5:FA:293:PHE:HZ | 5:FA:366:PRO:O | 2.00 | 0.43 |
| 5:FA:357:SER:HB3 | 5:FA:358:VAL:H | 1.55 | 0.43 |
| 6:FB:47:PHE:HE2 | 6:FB:51:ASN:HB3 | 1.84 | 0.43 |
| 6:FB:57:ASN:HB2 | 6:FC:164:GLN:NE2 | 2.33 | 0.43 |
| 7:FE:32:VAL:O | 7:FE:36:ILE:HG12 | 2.18 | 0.43 |
| 7:FE:44:VAL:HG21 | 7:FF:25:PHE:HB3 | 2.01 | 0.43 |
| 7:FF:126:ASN:O | 7:FF:129:PHE:HB3 | 2.18 | 0.43 |
| 7:FF:12:GLU:CG | 7:FF:15:TYR:H | 2.31 | 0.43 |
| 7:FG:182:THR:O | 7:FG:189:GLY:HA3 | 2.18 | 0.43 |
| 10:GA:203:ARG:NH1 | 10:GA:311:PHE:HE1 | 2.16 | 0.43 |
| 11:GB:107:ASP:HA | 11:GB:155:THR:HG22 | 2.00 | 0.43 |
| 1:GD:172:ILE:HD13 | 1:GD:273:ILE:HG12 | 1.99 | 0.43 |
| 1:GD:432:SER:O | 1:GD:435:TRP:HB3 | 2.18 | 0.43 |
| 1:GD:38:ASN:N | 1:GD:48:PHE:HE2 | 2.17 | 0.43 |
| 1:GE:373:PHE:O | 1:GE:374:ILE:HD13 | 2.18 | 0.43 |
| 1:GE:41:ASN:O | 1:GE:42:GLU:HG2 | 2.18 | 0.43 |
| 1:GE:559:ALA:HB3 | 1:GE:562:ASP:OD2 | 2.18 | 0.43 |
| 1:GE:485:VAL:HG22 | 1:GE:624:TYR:HD1 | 1.83 | 0.43 |
| 2:GF:151:PHE:HB3 | 2:GF:166:PHE:HZ | 1.83 | 0.43 |
| 2:GF:194:GLU:HG2 | 2:GF:199:LEU:HA | 2.01 | 0.43 |
| 2:GF:84:THR:O | 2:GF:91:GLN:NE2 | 2.51 | 0.43 |
| 2:GF:948:THR:HB | 2:GF:950:GLU:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:232:GLN:O | 3:GH:233:GLN:HB2 | 2.18 | 0.43 |
| 5:HC:410:GLN:HG3 | 5:HD:406:LEU:O | 2.18 | 0.43 |
| 6:HE:19:GLY:H | 6:HF:13:ARG:CZ | 2.30 | 0.43 |
| 5:HD:318:GLN:HB3 | 6:HF:4:LEU:CD1 | 2.48 | 0.43 |
| 6:HG:47:PHE:HE2 | 6:HG:51:ASN:HB3 | 1.84 | 0.43 |
| 7:HH:329:ASN:OD1 | 7:HH:330:ARG:N | 2.50 | 0.43 |
| 5:HD:196:ARG:HH11 | 7:HI:8:HIS:HB3 | 1.81 | 0.43 |
| 7:HJ:197:ALA:O | 7:HJ:201:GLN:HG3 | 2.18 | 0.43 |
| 7:HJ:272:GLN:NE2 | 7:HJ:277:ALA:HA | 2.33 | 0.43 |
| 5:HC:196:ARG:HH22 | 7:HJ:9:VAL:HG12 | 1.81 | 0.43 |
| 5:I:181:PHE:HE2 | 5:I:246:THR:HG22 | 1.83 | 0.43 |
| 5:I:323:THR:CG2 | 5:I:359:GLU:HB2 | 2.48 | 0.43 |
| 5:I:469:PRO:HA | 5:I:472:TYR:CZ | 2.54 | 0.43 |
| 5:I:49:TRP:HB2 | 5:K:90:ASN:OD1 | 2.17 | 0.43 |
| 5:J:363:ASN:N | 5:J:367:GLU:OE2 | 2.49 | 0.43 |
| 5:J:395:THR:OG1 | 5:J:396:LYS:N | 2.52 | 0.43 |
| 5:J:7:ILE:HD11 | 5:K:24:ILE:HD11 | 1.99 | 0.43 |
| 6:M:130:ARG:O | 6:M:134:GLN:HG3 | 2.18 | 0.43 |
| 7:O:163:LEU:HD23 | 7:O:167:GLN:HB2 | 2.01 | 0.43 |
| 7:P:117:THR:HB | 7:Q:112:ASN:HA | 2.00 | 0.43 |
| 7:P:118:PRO:HB3 | 7:Q:106:ALA:O | 2.19 | 0.43 |
| 7:Q:12:GLU:HG3 | 7:Q:15:TYR:H | 1.82 | 0.43 |
| 7:Q:161:THR:H | 7:Q:164:LYS:HB2 | 1.83 | 0.43 |
| 7:Q:197:ALA:O | 7:Q:201:GLN:HG3 | 2.18 | 0.43 |
| 7:Q:232:THR:HG23 | 7:Q:234:SER:N | 2.34 | 0.43 |
| 7:O:472:ARG:NH1 | 7:Q:474:GLY:HA2 | 2.33 | 0.43 |
| 7:Q:489:GLU:CD | 7:Q:502:LEU:H | 2.22 | 0.43 |
| 9:T:20:ASN:C | 9:T:20:ASN:OD1 | 2.57 | 0.43 |
| 9:T:7:LEU:HD23 | 9:T:7:LEU:HA | 1.78 | 0.43 |
| 12:W:99:SER:HB3 | 12:W:102:GLY:O | 2.17 | 0.43 |
| 1:X:336:GLN:HG3 | 1:X:337:GLN:N | 2.32 | 0.43 |
| 1:Y:55:VAL:HG21 | 2:Z:657:TYR:CZ | 2.54 | 0.43 |
| 13:YA:127[B]:ASN:ND2 | 13:YA:129[B]:THR:OG1 | 2.52 | 0.43 |
| 13:YA:263[B]:GLY:N | 13:YA:264[B]:PRO:HD2 | 2.33 | 0.43 |
| 13:YA:320[A]:THR:HG22 | 13:YA:323[A]:ARG:HB3 | 2.00 | 0.43 |
| 13:YA:471[D]:LEU:O | 13:YB:463[D]:ILE:HA | 2.18 | 0.43 |
| 13:YA:490[A]:VAL:HG12 | 13:YA:492[A]:GLY:H | 1.82 | 0.43 |
| 13:YA:544[A]:TRP:HB2 | 13:YC:552[A]:GLU:HB2 | 2.00 | 0.43 |
| 13:YA:565[F]:TYR:CZ | 13:YB:557[F]:MET:HG2 | 2.53 | 0.43 |
| 13:YA:70[D]:GLY:O | 13:YB:394[D]:GLU:N | 2.52 | 0.43 |
| 13:YA:9[E]:ASN:ND2 | 13:YC:7[E]:ASN:OD1 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:36[F]:PRO:HB2 | 13:YB:38[F]:GLN:OE1 | 2.17 | 0.43 |
| 13:YB:132[F]:LEU:O | 13:YB:390[F]:VAL:HG11 | 2.19 | 0.43 |
| 13:YA:70[C]:GLY:O | 13:YB:394[C]:GLU:N | 2.52 | 0.43 |
| 13:YB:50[B]:GLU:N | 13:YB:50[B]:GLU:CD | 2.71 | 0.43 |
| 13:YB:553[F]:LYS:HZ2 | 13:YB:553[F]:LYS:HB2 | 1.83 | 0.43 |
| 13:YB:564[C]:GLN:HG3 | 13:YB:566[C]:THR:HG22 | 2.01 | 0.43 |
| 13:YB:66[F]:MET:HE3 | 13:YB:66[F]:MET:HA | 1.99 | 0.43 |
| 13:YC:112[C]:GLU:C | 13:YC:115[C]:SER:HB3 | 2.38 | 0.43 |
| 13:YC:127[B]:ASN:ND2 | 13:YC:129[B]:THR:OG1 | 2.52 | 0.43 |
| 13:YC:127[C]:ASN:ND2 | 13:YC:129[C]:THR:OG1 | 2.52 | 0.43 |
| 13:YC:127[F]:ASN:ND2 | 13:YC:129[F]:THR:OG1 | 2.52 | 0.43 |
| 13:YC:147[A]:ILE:HD11 | 13:YC:188[A]:LEU:HG | 2.00 | 0.43 |
| 13:YC:200[E]:ILE:HD13 | 13:YC:236[E]:ILE:HD12 | 2.00 | 0.43 |
| 13:YC:236[A]:ILE:HG23 | 13:YC:240[A]:GLU:HB2 | 2.00 | 0.43 |
| 13:YC:263[B]:GLY:N | 13:YC:264[B]:PRO:HD2 | 2.33 | 0.43 |
| 13:YC:263[D]:GLY:N | 13:YC:264[D]:PRO:HD2 | 2.33 | 0.43 |
| 13:YC:304[C]:TRP:O | 13:YC:308[C]:TYR:N | 2.33 | 0.43 |
| 13:YC:327[E]:VAL:O | 13:YC:331[E]:ILE:HG22 | 2.19 | 0.43 |
| 13:YC:330[F]:ILE:HD12 | 13:YC:336[F]:LEU:HD12 | 2.00 | 0.43 |
| 13:YA:438[B]:LEU:CD2 | 13:YC:442[B]:THR:HG21 | 2.48 | 0.43 |
| 13:YB:476[F]:GLY:HA3 | 13:YC:469[F]:ASN:HA | 2.00 | 0.43 |
| 13:YB:60[B]:PRO:HB3 | 13:YC:60[B]:PRO:HB3 | 2.00 | 0.43 |
| 13:YB:92[A]:THR:HB | 14:YE:282[A]:ALA:CB | 2.49 | 0.43 |
| 14:YE:308[E]:ALA:O | 14:YE:357[E]:MET:N | 2.51 | 0.43 |
| 14:YE:80[B]:ILE:H | 14:YE:80[B]:ILE:HD13 | 1.83 | 0.43 |
| 14:YE:75[F]:ALA:HB2 | 14:YE:83[F]:VAL:HA | 2.00 | 0.43 |
| 14:YE:73[C]:SER:HA | 14:YE:85[C]:THR:HA | 2.00 | 0.43 |
| 14:YF:109[A]:LEU:HA | 14:YF:109[A]:LEU:HD12 | 1.65 | 0.43 |
| 13:YC:47[E]:ILE:HG12 | 14:YF:123[E]:PRO:HD3 | 2.01 | 0.43 |
| 14:YF:132[E]:ILE:HD12 | 14:YF:197[E]:MET:SD | 2.59 | 0.43 |
| 14:YF:88[A]:TYR:HD1 | 14:YF:110[A]:GLY:C | 2.21 | 0.43 |
| 14:YF:88[F]:TYR:HD1 | 14:YF:110[F]:GLY:C | 2.22 | 0.43 |
| 2:Z:1005:ARG:HG2 | 2:Z:1006:ASP:O | 2.19 | 0.43 |
| 2:Z:114:ILE:HG23 | 2:Z:115:GLU:N | 2.33 | 0.43 |
| 2:Z:151:PHE:HB3 | 2:Z:166:PHE:HZ | 1.83 | 0.43 |
| 2:Z:480:LEU:CD2 | 2:Z:488:MET:HB2 | 2.49 | 0.43 |
| 2:Z:478:GLU:HG3 | 2:Z:488:MET:SD | 2.58 | 0.43 |
| 2:Z:548:ILE:HG21 | 2:Z:555:ARG:H | 1.84 | 0.43 |
| 2:Z:937:THR:HA | 2:Z:941:GLU:O | 2.19 | 0.43 |
| 2:Z:9:THR:OG1 | 2:Z:10:SER:N | 2.51 | 0.43 |
| 1:A:557:PRO:HB3 | 1:A:589:TYR:CZ | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:AA:107:VAL:O | 4:AA:148:LEU:N | 2.39 | 0.43 |
| 5:AC:204:ASP:OD1 | 5:AC:205:VAL:N | 2.50 | 0.43 |
| 5:AC:326:MET:HB2 | 5:AC:326:MET:HE3 | 1.78 | 0.43 |
| 5:AC:323:THR:CG2 | 5:AC:354:THR:HG23 | 2.48 | 0.43 |
| 5:AD:421:ASN:HB2 | 5:AD:434:GLU:CG | 2.49 | 0.43 |
| 7:AI:102:THR:O | 7:AI:105:GLU:N | 2.52 | 0.43 |
| 7:AI:32:VAL:O | 7:AI:36:ILE:HG12 | 2.18 | 0.43 |
| 7:AI:95:TYR:HD1 | 7:BA:99:ARG:N | 2.17 | 0.43 |
| 7:AJ:228:ILE:O | 7:BA:226:GLY:N | 2.49 | 0.43 |
| 7:AJ:267:THR:O | 7:AJ:285:ALA:HA | 2.19 | 0.43 |
| 7:AJ:375:TYR:CZ | 7:AJ:392:LEU:HD23 | 2.53 | 0.43 |
| 7:AJ:451:PHE:HZ | 7:AJ:471:THR:HG22 | 1.82 | 0.43 |
| 1:B:116:ASP:HB2 | 1:B:161:TYR:HE2 | 1.84 | 0.43 |
| 1:B:206:TRP:CG | 1:B:222:THR:HB | 2.53 | 0.43 |
| 1:B:256:TYR:CD1 | 1:B:256:TYR:N | 2.83 | 0.43 |
| 9:BD:10:ASP:O | 9:BD:26:SER:N | 2.48 | 0.43 |
| 12:BG:164:MET:HB3 | 12:BG:237:THR:HG22 | 2.01 | 0.43 |
| 1:BH:430:GLN:H | 1:BH:430:GLN:CD | 2.14 | 0.43 |
| 1:BI:122:TYR:HB3 | 1:BI:152:ILE:HD11 | 2.01 | 0.43 |
| 1:BI:213:SER:HA | 2:BJ:733:ASP:CG | 2.38 | 0.43 |
| 1:BI:256:TYR:CD1 | 1:BI:256:TYR:N | 2.83 | 0.43 |
| 2:BJ:186:ASP:HB3 | 2:BJ:189:ARG:CD | 2.49 | 0.43 |
| 2:C:114:ILE:HG23 | 2:C:115:GLU:N | 2.33 | 0.43 |
| 2:C:321:VAL:HA | 2:C:326:VAL:HA | 2.01 | 0.43 |
| 4:CC:209:VAL:HG13 | 4:CC:271:GLY:O | 2.19 | 0.43 |
| 5:CF:469:PRO:HA | 5:CF:472:TYR:CZ | 2.54 | 0.43 |
| 5:CF:64:TRP:CZ2 | 5:CF:82:PRO:HB2 | 2.54 | 0.43 |
| 5:CH:130:PHE:HD2 | 5:CH:152:ASP:HB2 | 1.83 | 0.43 |
| 5:CH:89:TYR:CE1 | 5:CH:139:ALA:HA | 2.54 | 0.43 |
| 6:CI:88:TRP:O | 6:CI:155:LYS:HA | 2.18 | 0.43 |
| 6:DA:88:TRP:O | 6:DA:155:LYS:HA | 2.18 | 0.43 |
| 7:DB:183:ALA:O | 7:DB:184:THR:HG23 | 2.19 | 0.43 |
| 7:DC:458:GLY:O | 7:DC:461:GLY:N | 2.41 | 0.43 |
| 7:DC:451:PHE:HZ | 7:DC:471:THR:HG22 | 1.82 | 0.43 |
| 7:DD:134:SER:HB3 | 7:DD:140:GLY:N | 2.33 | 0.43 |
| 7:DD:232:THR:HG23 | 7:DD:234:SER:N | 2.34 | 0.43 |
| 7:DD:240:ASN:HB3 | 7:DD:243:VAL:HG22 | 2.00 | 0.43 |
| 7:DB:401:ARG:NH2 | 7:DD:397:GLY:O | 2.51 | 0.43 |
| 7:DC:477:TRP:CZ3 | 7:DD:469:VAL:HB | 2.53 | 0.43 |
| 3:E:265:GLY:HA3 | 1:Y:656:GLU:OE2 | 2.19 | 0.43 |
| 1:EA:209:TRP:CD1 | 1:EA:225:TYR:HE1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:116:ASP:HB2 | 1:EB:161:TYR:HE2 | 1.84 | 0.43 |
| 1:EB:154:ILE:HG22 | 1:EB:155:ARG:O | 2.19 | 0.43 |
| 1:EB:539:ARG:O | 1:EB:541:VAL:HG23 | 2.19 | 0.43 |
| 2:EC:511:GLU:N | 2:EC:512:PRO:HD2 | 2.32 | 0.43 |
| 2:EC:145:ALA:O | 2:EC:586:LEU:HB3 | 2.18 | 0.43 |
| 2:EC:934:ALA:H | 2:EC:997:SER:CB | 2.31 | 0.43 |
| 2:EC:947:VAL:HB | 3:ED:119:TYR:HB3 | 2.00 | 0.43 |
| 3:EE:175:ASP:OD1 | 3:EE:176:ALA:N | 2.48 | 0.43 |
| 3:EE:71:MET:SD | 3:EE:312:MET:HG2 | 2.58 | 0.43 |
| 5:EI:129:ARG:HG3 | 5:EI:130:PHE:N | 2.30 | 0.43 |
| 5:EI:323:THR:HG21 | 5:EI:354:THR:HA | 2.00 | 0.43 |
| 2:EC:1002:ALA:HA | 5:EJ:20:ARG:HB2 | 1.99 | 0.43 |
| 5:EJ:328:LEU:HG | 5:EJ:329:PHE:H | 1.84 | 0.43 |
| 5:EI:472:TYR:O | 5:EJ:416:ILE:HD12 | 2.18 | 0.43 |
| 5:EJ:466:PRO:HA | 5:EJ:596:TYR:CZ | 2.52 | 0.43 |
| 5:EJ:7:ILE:HD11 | 5:FA:24:ILE:HD11 | 2.01 | 0.43 |
| 5:EI:98:VAL:HG22 | 5:FA:90:ASN:HA | 2.00 | 0.43 |
| 6:FB:108:LEU:HD23 | 6:FB:113:PRO:HA | 2.00 | 0.43 |
| 6:FB:201:VAL:N | 6:FB:210:THR:O | 2.31 | 0.43 |
| 6:FC:172:SER:HA | 6:FC:176:ILE:O | 2.17 | 0.43 |
| 6:FD:64:ILE:HG23 | 6:FD:217:ARG:HH12 | 1.84 | 0.43 |
| 7:FE:176:ILE:HG23 | 7:FE:177:ALA:H | 1.84 | 0.43 |
| 7:FE:183:ALA:O | 7:FE:184:THR:HG23 | 2.19 | 0.43 |
| 7:FE:39:ILE:HG22 | 7:FG:44:VAL:CG2 | 2.49 | 0.43 |
| 7:FF:103:ASN:OD1 | 7:FF:120:LYS:HG2 | 2.19 | 0.43 |
| 7:FF:77:THR:CG2 | 7:FF:80:THR:H | 2.31 | 0.43 |
| 7:FE:99:ARG:N | 7:FF:95:TYR:HD1 | 2.16 | 0.43 |
| 7:FG:218:SER:O | 7:FG:227:VAL:HG22 | 2.19 | 0.43 |
| 7:FF:399:PHE:CD1 | 7:FG:401:ARG:HB3 | 2.52 | 0.43 |
| 4:G:209:VAL:HG13 | 4:G:271:GLY:O | 2.19 | 0.43 |
| 1:GD:278:ALA:HB2 | 1:GD:317:GLY:N | 2.33 | 0.43 |
| 1:GD:345:TYR:OH | 1:GD:400:ASN:ND2 | 2.51 | 0.43 |
| 1:GD:595:ILE:HG21 | 1:GD:602:ILE:HG23 | 1.99 | 0.43 |
| 1:GD:510:MET:HE3 | 1:GD:623:LEU:HD11 | 2.00 | 0.43 |
| 1:GE:256:TYR:CD1 | 1:GE:256:TYR:N | 2.83 | 0.43 |
| 1:GE:521:ARG:HB2 | 1:GE:533:ASP:CG | 2.39 | 0.43 |
| 1:GE:533:ASP:OD1 | 1:GE:534:VAL:HG22 | 2.18 | 0.43 |
| 2:GF:494:GLU:HB2 | 2:GF:498:TRP:CB | 2.49 | 0.43 |
| 3:GH:71:MET:SD | 3:GH:312:MET:HG2 | 2.58 | 0.43 |
| 4:GJ:190:PRO:HA | 4:GJ:262:THR:HA | 2.01 | 0.43 |
| 4:HA:209:VAL:HG13 | 4:HA:271:GLY:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:323:THR:HG21 | 5:HB:354:THR:HA | 2.00 | 0.43 |
| 5:HB:320:LEU:HG | 5:HB:357:SER:CB | 2.49 | 0.43 |
| 5:HD:180:VAL:HG22 | 5:HD:181:PHE:H | 1.84 | 0.43 |
| 5:HD:176:ASP:HA | 5:HD:231:ARG:HA | 1.99 | 0.43 |
| 5:HD:371:PHE:HZ | 5:HD:373:SER:HB3 | 1.83 | 0.43 |
| 5:HD:79:ILE:HD12 | 5:HD:81:LEU:HD11 | 2.01 | 0.43 |
| 5:HD:89:TYR:CE1 | 5:HD:139:ALA:HA | 2.54 | 0.43 |
| 7:P:167:GLN:CG | 6:HE:77:VAL:HG23 | 2.48 | 0.43 |
| 6:HF:47:PHE:HE2 | 6:HF:51:ASN:HB3 | 1.84 | 0.43 |
| 7:HH:163:LEU:HD23 | 7:HH:167:GLN:HB2 | 2.01 | 0.43 |
| 7:HI:118:PRO:HB3 | 7:HJ:106:ALA:O | 2.19 | 0.43 |
| 7:HI:20:PRO:HB3 | 7:HI:29:ILE:HG13 | 2.01 | 0.43 |
| 7:HJ:14:ARG:HG2 | 7:HJ:33:GLN:HG2 | 2.01 | 0.43 |
| 7:HJ:29:ILE:HG22 | 7:HJ:30:THR:N | 2.18 | 0.43 |
| 7:HH:408:HIS:CE1 | 7:HJ:437:VAL:HG21 | 2.53 | 0.43 |
| 5:I:279:SER:HB2 | 5:K:326:MET:HB2 | 2.00 | 0.43 |
| 5:I:322:GLY:HA2 | 5:I:360:THR:N | 2.34 | 0.43 |
| 5:I:90:ASN:HD21 | 5:J:49:TRP:C | 2.18 | 0.43 |
| 9:IC:20:ASN:C | 9:IC:20:ASN:OD1 | 2.57 | 0.43 |
| 11:IE:73:LEU:HD22 | 11:IE:86:TRP:CH2 | 2.52 | 0.43 |
| 5:K:130:PHE:HD2 | 5:K:152:ASP:HB2 | 1.83 | 0.43 |
| 5:K:371:PHE:HZ | 5:K:373:SER:HB3 | 1.84 | 0.43 |
| 5:I:407:TYR:CD1 | 5:K:407:TYR:HB2 | 2.53 | 0.43 |
| 5:I:408:VAL:HG23 | 5:K:409:SER:O | 2.19 | 0.43 |
| 6:L:108:LEU:HD23 | 6:L:113:PRO:HA | 2.00 | 0.43 |
| 6:L:47:PHE:HE2 | 6:L:51:ASN:HB3 | 1.84 | 0.43 |
| 6:N:64:ILE:HG23 | 6:N:217:ARG:HH12 | 1.84 | 0.43 |
| 7:P:342:PRO:HB2 | 7:P:378:ARG:HH12 | 1.83 | 0.43 |
| 7:P:46:GLY:O | 7:P:47:VAL:HG23 | 2.19 | 0.43 |
| 7:P:480:ARG:CZ | 7:Q:465:ARG:HG3 | 2.48 | 0.43 |
| 7:Q:182:THR:O | 7:Q:189:GLY:HA3 | 2.18 | 0.43 |
| 7:Q:20:PRO:CG | 7:Q:29:ILE:HG13 | 2.49 | 0.43 |
| 7:Q:58:LEU:HD21 | 7:Q:75:ALA:H | 1.84 | 0.43 |
| 12:W:117:ALA:O | 12:W:120:SER:OG | 2.24 | 0.43 |
| 1:X:525:ASN:HB3 | 1:X:528:THR:CG2 | 2.48 | 0.43 |
| 1:Y:199:LEU:HD21 | 1:Y:224:TYR:CG | 2.53 | 0.43 |
| 1:Y:429:LEU:O | 1:Y:429:LEU:HD12 | 2.19 | 0.43 |
| 1:Y:448:TYR:HA | 1:Y:452:VAL:CG1 | 2.49 | 0.43 |
| 13:YA:112[C]:GLU:C | 13:YA:115[C]:SER:HB3 | 2.39 | 0.43 |
| 13:YA:127[C]:ASN:ND2 | 13:YA:129[C]:THR:OG1 | 2.52 | 0.43 |
| 13:YA:147[E]:ILE:HD11 | 13:YA:188[E]:LEU:HG | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:200[D]:ILE:HD13 | 13:YA:236[D]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:24[A]:LEU:HA | 13:YA:24[A]:LEU:HD12 | 1.63 | 0.43 |
| 13:YA:263[F]:GLY:N | 13:YA:264[F]:PRO:HD2 | 2.33 | 0.43 |
| 13:YA:552[B]:GLU:CG | 13:YA:554[B]:MET:HE1 | 2.48 | 0.43 |
| 13:YA:565[A]:TYR:CZ | 13:YB:557[A]:MET:HG2 | 2.53 | 0.43 |
| 13:YA:564[E]:GLN:HG3 | 13:YA:566[E]:THR:HG22 | 2.01 | 0.43 |
| 13:YA:76[E]:PRO:C | 13:YC:61[E]:ILE:HG22 | 2.39 | 0.43 |
| 13:YB:236[A]:ILE:HG23 | 13:YB:240[A]:GLU:HB2 | 1.99 | 0.43 |
| 13:YB:263[D]:GLY:N | 13:YB:264[D]:PRO:HD2 | 2.33 | 0.43 |
| 13:YB:263[F]:GLY:N | 13:YB:264[F]:PRO:HD2 | 2.33 | 0.43 |
| 13:YB:278[C]:GLU:O | 13:YB:282[C]:PHE:N | 2.52 | 0.43 |
| 13:YB:327[B]:VAL:O | 13:YB:331[B]:ILE:HG22 | 2.19 | 0.43 |
| 13:YB:476[B]:GLY:HA3 | 13:YC:469[B]:ASN:HA | 2.00 | 0.43 |
| 13:YA:565[E]:TYR:CZ | 13:YB:557[E]:MET:HG2 | 2.53 | 0.43 |
| 13:YA:61[F]:ILE:HG12 | 13:YB:60[F]:PRO:HD3 | 2.00 | 0.43 |
| 13:YA:473[A]:GLN:OE1 | 13:YC:158[A]:PRO:HB2 | 2.18 | 0.43 |
| 13:YC:327[B]:VAL:O | 13:YC:331[B]:ILE:HG22 | 2.19 | 0.43 |
| 13:YA:438[C]:LEU:CD2 | 13:YC:442[C]:THR:HG21 | 2.48 | 0.43 |
| 13:YA:452[B]:GLY:O | 13:YC:460[B]:GLY:N | 2.51 | 0.43 |
| 13:YA:452[F]:GLY:O | 13:YC:460[F]:GLY:N | 2.52 | 0.43 |
| 13:YB:530[D]:VAL:HG22 | 13:YC:522[D]:VAL:HG13 | 2.01 | 0.43 |
| 13:YC:534[A]:LEU:HD11 | 13:YC:536[A]:TRP:NE1 | 2.32 | 0.43 |
| 13:YC:552[D]:GLU:CG | 13:YC:554[D]:MET:HE1 | 2.48 | 0.43 |
| 13:YA:551[E]:THR:HA | 13:YC:558[E]:SER:O | 2.18 | 0.43 |
| 13:YC:564[E]:GLN:HG3 | 13:YC:566[E]:THR:HG22 | 2.01 | 0.43 |
| 13:YA:9[F]:ASN:ND2 | 13:YC:7[F]:ASN:OD1 | 2.51 | 0.43 |
| 14:YD:132[A]:ILE:HD12 | 14:YD:197[A]:MET:SD | 2.59 | 0.43 |
| 14:YD:132[F]:ILE:HD12 | 14:YD:197[F]:MET:SD | 2.59 | 0.43 |
| 14:YD:172[D]:TYR:CZ | 14:YD:176[D]:VAL:HG21 | 2.54 | 0.43 |
| 14:YD:172[A]:TYR:CZ | 14:YD:176[A]:VAL:HG21 | 2.54 | 0.43 |
| 14:YD:86[D]:ARG:HD2 | 14:YD:192[D]:ILE:HD12 | 2.00 | 0.43 |
| 14:YD:288[C]:TYR:CE1 | 14:YD:371[C]:LYS:HD3 | 2.53 | 0.43 |
| 14:YD:373[D]:LYS:HB3 | 14:YD:373[D]:LYS:HE2 | 1.87 | 0.43 |
| 14:YD:80[C]:ILE:HD13 | 14:YD:80[C]:ILE:H | 1.83 | 0.43 |
| 14:YD:86[A]:ARG:HD2 | 14:YD:192[A]:ILE:HD12 | 2.01 | 0.43 |
| 14:YE:132[A]:ILE:HD12 | 14:YE:197[A]:MET:SD | 2.59 | 0.43 |
| 14:YE:132[C]:ILE:HD12 | 14:YE:197[C]:MET:SD | 2.58 | 0.43 |
| 14:YE:172[E]:TYR:CZ | 14:YE:176[E]:VAL:HG21 | 2.54 | 0.43 |
| 14:YE:17[F]:PHE:HE2 | 14:YE:26[F]:ASN:HA | 1.83 | 0.43 |
| 14:YE:233[B]:ASP:N | 14:YE:233[B]:ASP:OD1 | 2.51 | 0.43 |
| 13:YB:26[F]:ARG:HD3 | 14:YE:259[F]:LEU:HD21 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:44[D]:LEU:HB2 | 14:YE:340[D]:ASP:O | 2.18 | 0.43 |
| 14:YE:80[A]:ILE:HD13 | 14:YE:80[A]:ILE:H | 1.83 | 0.43 |
| 14:YE:80[C]:ILE:HD13 | 14:YE:80[C]:ILE:H | 1.83 | 0.43 |
| 14:YF:15[D]:LYS:HE2 | 14:YF:15[D]:LYS:HB3 | 1.53 | 0.43 |
| 14:YF:44[A]:LEU:HB2 | 14:YF:340[A]:ASP:O | 2.18 | 0.43 |
| 14:YF:44[B]:LEU:HB2 | 14:YF:340[B]:ASP:O | 2.18 | 0.43 |
| 14:YF:80[E]:ILE:HD13 | 14:YF:80[E]:ILE:H | 1.83 | 0.43 |
| 14:YE:242[A]:PRO:HD2 | 14:YF:91[A]:LYS:O | 2.19 | 0.43 |
| 2:Z:194:GLU:HG2 | 2:Z:199:LEU:HA | 2.01 | 0.43 |
| 2:Z:213:ASN:HB2 | 2:Z:289:PHE:CZ | 2.53 | 0.43 |
| 15:ZA:37[A]:LEU:HB2 | 15:ZA:75[A]:VAL:HB | 2.01 | 0.43 |
| 4:AB:145:LYS:N | 4:AB:165:GLU:O | 2.49 | 0.43 |
| 4:AB:209:VAL:HG13 | 4:AB:271:GLY:O | 2.19 | 0.43 |
| 5:AC:288:MET:HG2 | 5:AC:289:LYS:O | 2.18 | 0.43 |
| 5:AD:285:LEU:HD21 | 5:AD:375:PHE:N | 2.21 | 0.43 |
| 5:AD:326:MET:HB2 | 5:AD:326:MET:HE3 | 1.65 | 0.43 |
| 5:AE:49:TRP:CZ3 | 5:AE:96:ARG:HD2 | 2.54 | 0.43 |
| 6:AF:6:ASN:HB3 | 6:AG:12:SER:CB | 2.49 | 0.43 |
| 6:AH:91:SER:OG | 6:AH:177:THR:HB | 2.18 | 0.43 |
| 7:AI:111:ASN:ND2 | 7:AI:114:SER:HB3 | 2.34 | 0.43 |
| 7:AI:190:VAL:HB | 7:AJ:188:GLN:C | 2.39 | 0.43 |
| 7:AI:472:ARG:NH1 | 7:BA:474:GLY:HA2 | 2.34 | 0.43 |
| 7:AI:13:SER:CB | 7:AJ:18:PHE:HA | 2.44 | 0.43 |
| 1:B:352:ARG:HD2 | 1:B:352:ARG:HA | 1.82 | 0.43 |
| 1:B:72:ASN:HB3 | 11:V:28:ILE:HG23 | 2.00 | 0.43 |
| 7:BA:232:THR:HG23 | 7:BA:234:SER:N | 2.34 | 0.43 |
| 7:BA:14:ARG:HG2 | 7:BA:33:GLN:HG2 | 2.01 | 0.43 |
| 8:BB:5:ASP:HA | 8:BB:8:ARG:HB3 | 2.00 | 0.43 |
| 8:BB:3:VAL:HG12 | 8:BC:58:ILE:HG23 | 2.00 | 0.43 |
| 10:BE:225:ILE:HG21 | 10:BE:225:ILE:HD13 | 1.77 | 0.43 |
| 12:BG:153:ARG:NH2 | 12:DJ:184:PRO:HA | 2.34 | 0.43 |
| 1:BH:655:LEU:O | 1:BH:655:LEU:HD12 | 2.19 | 0.43 |
| 1:BI:154:ILE:HG22 | 1:BI:155:ARG:O | 2.19 | 0.43 |
| 1:BI:116:ASP:HB2 | 1:BI:161:TYR:HE2 | 1.84 | 0.43 |
| 1:BI:521:ARG:HB2 | 1:BI:533:ASP:CG | 2.39 | 0.43 |
| 2:BJ:145:ALA:HB2 | 2:BJ:542:THR:CB | 2.48 | 0.43 |
| 2:BJ:168:ILE:HD12 | 2:BJ:168:ILE:HA | 1.88 | 0.43 |
| 2:C:151:PHE:HB3 | 2:C:166:PHE:HZ | 1.83 | 0.43 |
| 2:C:366:TYR:HB2 | 2:C:380:ILE:CD1 | 2.41 | 0.43 |
| 2:C:374:LYS:HB2 | 2:C:374:LYS:HE3 | 1.85 | 0.43 |
| 4:CC:124:ILE:HB | 4:CC:137:LEU:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CE:190:PRO:HA | 4:CE:262:THR:HA | 2.01 | 0.43 |
| 4:CE:209:VAL:HG13 | 4:CE:271:GLY:O | 2.19 | 0.43 |
| 5:CF:89:TYR:CD1 | 5:CF:139:ALA:HA | 2.54 | 0.43 |
| 5:CF:265:LEU:HD22 | 5:CF:281:TYR:HD2 | 1.84 | 0.43 |
| 5:CF:320:LEU:HG | 5:CF:357:SER:CB | 2.49 | 0.43 |
| 5:CF:89:TYR:CE1 | 5:CF:137:TYR:CZ | 3.06 | 0.43 |
| 5:CG:177:PHE:HD2 | 5:CG:230:ILE:HD11 | 1.83 | 0.43 |
| 5:CG:253:GLN:HB2 | 5:CG:255:ARG:HE | 1.84 | 0.43 |
| 5:CH:117:ILE:HG13 | 5:CH:118:LYS:H | 1.83 | 0.43 |
| 5:CH:340:VAL:HG21 | 6:CI:174:TYR:H | 1.83 | 0.43 |
| 5:CF:535:THR:OG1 | 5:CH:576:THR:HB | 2.18 | 0.43 |
| 5:CH:84:GLY:C | 5:CH:86:VAL:H | 2.17 | 0.43 |
| 3:D:150:LYS:HA | 3:D:160:TRP:CZ3 | 2.53 | 0.43 |
| 3:D:194:ILE:HG12 | 3:D:223:TRP:HZ3 | 1.84 | 0.43 |
| 3:D:279:LEU:HA | 3:D:279:LEU:HD23 | 1.76 | 0.43 |
| 6:CJ:7:LYS:HD3 | 6:DA:11:ILE:HA | 2.01 | 0.43 |
| 6:CJ:32:ARG:NH1 | 6:DA:144:ASN:OD1 | 2.44 | 0.43 |
| 7:DB:161:THR:HA | 7:DC:158:THR:O | 2.19 | 0.43 |
| 7:DB:26:PRO:HA | 7:DB:27:PRO:HD3 | 1.80 | 0.43 |
| 7:DB:519:LEU:HA | 7:DC:434:VAL:HG13 | 2.00 | 0.43 |
| 7:DC:103:ASN:OD1 | 7:DC:120:LYS:HG2 | 2.19 | 0.43 |
| 7:DB:509:GLY:O | 7:DC:443:SER:HA | 2.19 | 0.43 |
| 8:DF:21:PHE:CG | 8:FI:142:LEU:HD21 | 2.54 | 0.43 |
| 11:DI:31:ASN:O | 11:DI:32:TYR:HB2 | 2.18 | 0.43 |
| 12:DJ:118:TYR:CG | 12:DJ:119:ASN:N | 2.86 | 0.43 |
| 12:DJ:164:MET:HB3 | 12:DJ:237:THR:HG22 | 2.01 | 0.43 |
| 1:EA:38:ASN:N | 1:EA:48:PHE:HE2 | 2.17 | 0.43 |
| 1:EA:508:ARG:HH22 | 1:EA:577:PHE:HA | 1.84 | 0.43 |
| 1:EB:55:VAL:HG21 | 2:EC:657:TYR:CZ | 2.54 | 0.43 |
| 1:EB:66:TYR:O | 1:EB:70:PHE:N | 2.41 | 0.43 |
| 2:BJ:450:PHE:HE2 | 3:ED:70:ASP:OD2 | 2.01 | 0.43 |
| 3:EE:294:LYS:HB2 | 3:EE:297:TYR:CZ | 2.53 | 0.43 |
| 4:EF:124:ILE:HB | 4:EF:137:LEU:HB3 | 2.01 | 0.43 |
| 4:EG:192:PHE:CE1 | 4:EG:197:TYR:HB2 | 2.53 | 0.43 |
| 4:EH:124:ILE:HB | 4:EH:137:LEU:HB3 | 2.01 | 0.43 |
| 5:EI:320:LEU:HG | 5:EI:357:SER:CB | 2.49 | 0.43 |
| 5:EI:424:ASP:OD2 | 5:EI:427:LYS:HB3 | 2.19 | 0.43 |
| 5:EJ:129:ARG:HG3 | 5:EJ:130:PHE:N | 2.33 | 0.43 |
| 5:EJ:569:TYR:CD1 | 5:FA:544:VAL:HA | 2.53 | 0.43 |
| 5:FA:318:GLN:HB3 | 6:FC:4:LEU:CD1 | 2.49 | 0.43 |
| 5:FA:79:ILE:HD12 | 5:FA:81:LEU:HD11 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FB:88:TRP:O | 6:FB:155:LYS:HA | 2.18 | 0.43 |
| 6:FC:64:ILE:HG23 | 6:FC:217:ARG:HH12 | 1.84 | 0.43 |
| 6:FB:10:VAL:HG11 | 6:FD:10:VAL:HG21 | 2.01 | 0.43 |
| 6:FD:117:THR:H | 6:FD:120:MET:HE3 | 1.84 | 0.43 |
| 6:FD:130:ARG:O | 6:FD:134:GLN:HG3 | 2.18 | 0.43 |
| 7:FE:167:GLN:O | 7:FE:171:LYS:HG2 | 2.18 | 0.43 |
| 7:FE:408:HIS:CE1 | 7:FG:437:VAL:HG21 | 2.53 | 0.43 |
| 6:CI:213:TYR:OH | 7:FF:171:LYS:HG3 | 2.19 | 0.43 |
| 7:FF:46:GLY:O | 7:FF:47:VAL:HG23 | 2.19 | 0.43 |
| 7:FE:139:ASN:N | 7:FG:143:LYS:HG2 | 2.33 | 0.43 |
| 7:FG:168:LEU:HD23 | 7:FG:168:LEU:HA | 1.79 | 0.43 |
| 7:FE:288:ILE:HG13 | 7:FG:288:ILE:HG22 | 2.01 | 0.43 |
| 7:FE:407:SER:N | 7:FG:394:ASP:OD2 | 2.39 | 0.43 |
| 7:FG:417:ASN:HB3 | 7:FG:421:GLY:HA2 | 2.01 | 0.43 |
| 8:FH:15:PHE:N | 8:FH:15:PHE:CD1 | 2.84 | 0.43 |
| 8:FH:22:GLN:OE1 | 8:FH:116:TYR:OH | 2.25 | 0.43 |
| 8:FI:5:ASP:HA | 8:FI:8:ARG:HB3 | 2.00 | 0.43 |
| 10:GA:322:ASP:O | 10:GA:342:PHE:HB2 | 2.19 | 0.43 |
| 12:GC:18:ARG:HB2 | 12:GC:21:MET:HG2 | 2.01 | 0.43 |
| 1:GD:113:THR:O | 1:GD:298:ILE:HG13 | 2.18 | 0.43 |
| 1:GD:655:LEU:HD12 | 1:GD:655:LEU:O | 2.19 | 0.43 |
| 1:GE:330:THR:HG23 | 1:GE:333:ARG:HE | 1.83 | 0.43 |
| 1:GE:539:ARG:O | 1:GE:541:VAL:HG23 | 2.19 | 0.43 |
| 2:GF:145:ALA:O | 2:GF:586:LEU:HB3 | 2.18 | 0.43 |
| 2:GF:455:VAL:CG2 | 2:GF:472:LYS:HB3 | 2.49 | 0.43 |
| 2:GF:511:GLU:N | 2:GF:512:PRO:HD2 | 2.32 | 0.43 |
| 2:GF:613:LYS:O | 2:GF:615:THR:N | 2.47 | 0.43 |
| 2:GF:701:TRP:O | 2:GF:701:TRP:CG | 2.72 | 0.43 |
| 3:GG:294:LYS:N | 3:GG:297:TYR:OH | 2.43 | 0.43 |
| 3:GH:175:ASP:OD1 | 3:GH:176:ALA:N | 2.48 | 0.43 |
| 4:GJ:44:ASP:O | 4:GJ:59:GLN:NE2 | 2.52 | 0.43 |
| 4:H:124:ILE:HB | 4:H:137:LEU:HB3 | 2.01 | 0.43 |
| 4:HA:124:ILE:HB | 4:HA:137:LEU:HB3 | 2.01 | 0.43 |
| 5:HB:170:GLU:O | 5:HB:171:VAL:HG12 | 2.19 | 0.43 |
| 5:HB:323:THR:CG2 | 5:HB:359:GLU:HB2 | 2.48 | 0.43 |
| 5:HC:34:TYR:O | 5:HC:38:GLY:N | 2.37 | 0.43 |
| 5:HD:130:PHE:HD2 | 5:HD:152:ASP:HB2 | 1.83 | 0.43 |
| 5:HB:535:THR:OG1 | 5:HD:576:THR:HB | 2.18 | 0.43 |
| 7:HH:32:VAL:HG22 | 7:HH:36:ILE:HG12 | 2.01 | 0.43 |
| 5:CH:351:GLN:HG2 | 7:HH:467:ASN:ND2 | 2.34 | 0.43 |
| 7:HJ:425:LEU:HA | 7:HJ:425:LEU:HD23 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HJ:445:HIS:CD2 | 7:HJ:447:HIS:CE1 | 3.06 | 0.43 |
| 7:HJ:67:ILE:HA | 7:HJ:84:ARG:NH2 | 2.31 | 0.43 |
| 5:I:320:LEU:HG | 5:I:357:SER:CB | 2.49 | 0.43 |
| 5:I:394:LEU:HD22 | 5:K:395:THR:HA | 2.01 | 0.43 |
| 8:IB:134:PRO:HA | 8:IB:157:LEU:HD23 | 2.01 | 0.43 |
| 8:IB:98:GLU:OE1 | 8:IB:98:GLU:N | 2.48 | 0.43 |
| 10:U:290:PRO:HD3 | 10:ID:197:TYR:CZ | 2.54 | 0.43 |
| 10:ID:322:ASP:O | 10:ID:342:PHE:HB2 | 2.19 | 0.43 |
| 11:IE:43:TYR:O | 11:IE:44:ARG:HB2 | 2.19 | 0.43 |
| 5:J:323:THR:HG22 | 5:J:355:ASP:O | 2.18 | 0.43 |
| 5:J:261:ARG:N | 5:J:383:ILE:O | 2.34 | 0.43 |
| 5:J:569:TYR:HD1 | 5:K:544:VAL:HA | 1.83 | 0.43 |
| 5:K:79:ILE:HD12 | 5:K:81:LEU:HD11 | 2.01 | 0.43 |
| 6:L:88:TRP:O | 6:L:155:LYS:HA | 2.18 | 0.43 |
| 6:N:73:ASN:ND2 | 6:N:215:PHE:HE2 | 2.16 | 0.43 |
| 7:O:77:THR:HG22 | 7:O:80:THR:H | 1.83 | 0.43 |
| 7:O:143:LYS:HG2 | 7:P:138:SER:C | 2.39 | 0.43 |
| 7:P:197:ALA:CB | 6:HG:32:ARG:HA | 2.49 | 0.43 |
| 7:P:267:THR:O | 7:P:285:ALA:HA | 2.19 | 0.43 |
| 7:Q:349:TRP:NE1 | 7:Q:351:ALA:HB3 | 2.34 | 0.43 |
| 11:V:55:ARG:HD2 | 11:V:55:ARG:HA | 1.83 | 0.43 |
| 1:X:113:THR:O | 1:X:298:ILE:HG13 | 2.18 | 0.43 |
| 1:X:347:THR:O | 1:X:350:SER:N | 2.52 | 0.43 |
| 1:Y:122:TYR:HB3 | 1:Y:152:ILE:HD11 | 2.01 | 0.43 |
| 1:Y:240:GLU:HB2 | 2:Z:719:LYS:HZ1 | 1.84 | 0.43 |
| 1:Y:348:PHE:HZ | 1:Y:399:TYR:HD2 | 1.65 | 0.43 |
| 1:Y:371:TYR:HB3 | 1:Y:373:PHE:CE1 | 2.54 | 0.43 |
| 13:YA:195[D]:GLU:HG2 | 13:YA:197[D]:TYR:CE2 | 2.54 | 0.43 |
| 13:YA:200[C]:ILE:HD13 | 13:YA:236[C]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:200[A]:ILE:HD13 | 13:YA:236[A]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:200[F]:ILE:HD13 | 13:YA:236[F]:ILE:HD12 | 2.01 | 0.43 |
| 13:YA:363[F]:PRO:HB2 | 13:YC:284[F]:MET:HE3 | 2.01 | 0.43 |
| 13:YA:389[D]:TYR:O | 13:YA:405[D]:ASP:HB2 | 2.19 | 0.43 |
| 13:YA:560[D]:ILE:O | 13:YB:553[D]:LYS:HA | 2.19 | 0.43 |
| 13:YA:560[E]:ILE:O | 13:YB:553[E]:LYS:HA | 2.18 | 0.43 |
| 13:YA:564[C]:GLN:HG3 | 13:YA:566[C]:THR:HG22 | 2.01 | 0.43 |
| 13:YA:574[B]:ILE:O | 15:ZA:70[B]:THR:N | 2.27 | 0.43 |
| 13:YA:83[C]:TYR:OH | 13:YA:85[C]:HIS:HE1 | 2.02 | 0.43 |
| 13:YB:127[E]:ASN:ND2 | 13:YB:129[E]:THR:OG1 | 2.52 | 0.43 |
| 13:YB:154[B]:THR:H | 13:YB:182[B]:ARG:NH2 | 2.17 | 0.43 |
| 13:YB:154[E]:THR:H | 13:YB:182[E]:ARG:NH2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:278[E]:GLU:O | 13:YB:282[E]:PHE:N | 2.51 | 0.43 |
| 13:YB:278[D]:GLU:O | 13:YB:282[D]:PHE:N | 2.52 | 0.43 |
| 13:YB:330[A]:ILE:HD12 | 13:YB:336[A]:LEU:HD12 | 2.01 | 0.43 |
| 13:YB:327[E]:VAL:O | 13:YB:331[E]:ILE:HG22 | 2.19 | 0.43 |
| 13:YB:132[B]:LEU:O | 13:YB:390[B]:VAL:HG11 | 2.19 | 0.43 |
| 13:YA:551[F]:THR:O | 13:YB:543[F]:ASP:HA | 2.19 | 0.43 |
| 13:YB:58[C]:ILE:HG12 | 13:YB:97[C]:LEU:HD22 | 2.01 | 0.43 |
| 13:YC:127[E]:ASN:ND2 | 13:YC:129[E]:THR:OG1 | 2.52 | 0.43 |
| 13:YC:327[D]:VAL:O | 13:YC:331[D]:ILE:HG22 | 2.19 | 0.43 |
| 13:YC:132[E]:LEU:O | 13:YC:390[E]:VAL:HG11 | 2.19 | 0.43 |
| 13:YA:538[E]:VAL:O | 13:YC:546[E]:VAL:HA | 2.19 | 0.43 |
| 14:YD:88[C]:TYR:HD1 | 14:YD:110[C]:GLY:C | 2.21 | 0.43 |
| 14:YD:172[E]:TYR:CZ | 14:YD:176[E]:VAL:HG21 | 2.54 | 0.43 |
| 14:YD:38[C]:LEU:HA | 14:YD:38[C]:LEU:HD12 | 1.63 | 0.43 |
| 14:YD:44[F]:LEU:HB2 | 14:YD:340[F]:ASP:O | 2.18 | 0.43 |
| 14:YD:80[D]:ILE:H | 14:YD:80[D]:ILE:HD13 | 1.83 | 0.43 |
| 14:YD:73[E]:SER:HA | 14:YD:85[E]:THR:HA | 2.00 | 0.43 |
| 14:YD:86[B]:ARG:HD2 | 14:YD:192[B]:ILE:HD12 | 2.01 | 0.43 |
| 10:ID:286:VAL:HG13 | 14:YE:100[F]:LYS:CE | 2.49 | 0.43 |
| 14:YE:127[B]:ASP:CG | 14:YE:130[B]:GLU:H | 2.20 | 0.43 |
| 14:YE:86[E]:ARG:HD2 | 14:YE:192[E]:ILE:HD12 | 2.01 | 0.43 |
| 14:YE:233[C]:ASP:N | 14:YE:233[C]:ASP:OD1 | 2.51 | 0.43 |
| 14:YE:277[C]:VAL:HG11 | 14:YE:294[C]:GLU:HG2 | 1.99 | 0.43 |
| 14:YE:73[D]:SER:HA | 14:YE:85[D]:THR:HA | 2.01 | 0.43 |
| 14:YE:88[A]:TYR:HD1 | 14:YE:110[A]:GLY:C | 2.21 | 0.43 |
| 14:YF:172[A]:TYR:CZ | 14:YF:176[A]:VAL:HG21 | 2.54 | 0.43 |
| 14:YF:86[C]:ARG:HD2 | 14:YF:192[C]:ILE:HD12 | 2.01 | 0.43 |
| 14:YF:38[E]:LEU:HD12 | 14:YF:38[E]:LEU:HA | 1.63 | 0.43 |
| 14:YF:80[A]:ILE:HD13 | 14:YF:80[A]:ILE:H | 1.83 | 0.43 |
| 14:YF:80[F]:ILE:HD13 | 14:YF:80[F]:ILE:H | 1.83 | 0.43 |
| 2:Z:222:VAL:HG12 | 2:Z:224:LEU:HB2 | 2.01 | 0.43 |
| 2:Z:376:PHE:CZ | 2:Z:441:VAL:HG11 | 2.51 | 0.43 |
| 1:A:341:THR:HG23 | 2:C:880:ILE:O | 2.18 | 0.43 |
| 1:A:508:ARG:HH22 | 1:A:577:PHE:HA | 1.84 | 0.43 |
| 1:A:655:LEU:O | 1:A:655:LEU:HD12 | 2.19 | 0.43 |
| 5:AC:403:THR:HA | 5:AC:406:LEU:HB2 | 2.01 | 0.43 |
| 5:AD:341:GLU:C | 5:AD:343:SER:H | 2.22 | 0.43 |
| 5:AE:89:TYR:CE1 | 5:AE:139:ALA:HA | 2.54 | 0.43 |
| 5:AE:158:ASP:OD1 | 5:AE:159:ILE:N | 2.47 | 0.43 |
| 6:AF:73:ASN:ND2 | 6:AF:215:PHE:HE2 | 2.16 | 0.43 |
| 7:AI:183:ALA:O | 7:AI:184:THR:HG23 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:118:PRO:HB3 | 7:BA:106:ALA:O | 2.19 | 0.43 |
| 1:B:373:PHE:O | 1:B:374:ILE:HD13 | 2.18 | 0.43 |
| 1:B:41:ASN:O | 1:B:42:GLU:HG2 | 2.18 | 0.43 |
| 1:B:66:TYR:OH | 11:V:57:GLU:OE1 | 2.37 | 0.43 |
| 7:BA:111:ASN:ND2 | 7:BA:114:SER:HB3 | 2.34 | 0.43 |
| 7:BA:133:VAL:HA | 7:BA:141:VAL:O | 2.18 | 0.43 |
| 7:BA:182:THR:O | 7:BA:189:GLY:HA3 | 2.18 | 0.43 |
| 7:BA:26:PRO:HA | 7:BA:27:PRO:HD3 | 1.69 | 0.43 |
| 9:BD:33:LYS:HG2 | 9:BD:122:ILE:HG21 | 1.99 | 0.43 |
| 11:BF:2:LEU:HD23 | 11:BF:32:TYR:CD1 | 2.53 | 0.43 |
| 1:BH:90:VAL:HG11 | 1:BH:228:GLU:HG2 | 2.01 | 0.43 |
| 1:BH:494:THR:HG22 | 1:BH:498:GLY:HA2 | 2.01 | 0.43 |
| 2:BJ:186:ASP:HB3 | 2:BJ:189:ARG:HE | 1.83 | 0.43 |
| 2:BJ:653:MET:SD | 2:BJ:654:PRO:HD2 | 2.59 | 0.43 |
| 2:C:241:SER:O | 2:C:244:THR:OG1 | 2.25 | 0.43 |
| 2:C:455:VAL:CG2 | 2:C:472:LYS:HB3 | 2.48 | 0.43 |
| 2:C:450:PHE:HE2 | 2:C:473:TYR:HH | 1.66 | 0.43 |
| 2:C:494:GLU:HB2 | 2:C:498:TRP:CB | 2.49 | 0.43 |
| 4:CC:224:ASP:OD2 | 4:CC:227:ASN:HB2 | 2.19 | 0.43 |
| 4:CC:32:ASN:HD21 | 4:CD:10:ILE:HB | 1.84 | 0.43 |
| 4:CD:124:ILE:HB | 4:CD:137:LEU:HB3 | 2.01 | 0.43 |
| 4:CC:7:LYS:HD3 | 4:CE:39:TYR:CD2 | 2.54 | 0.43 |
| 5:CF:285:LEU:HD11 | 5:CF:375:PHE:CB | 2.41 | 0.43 |
| 5:CF:323:THR:HG21 | 5:CF:354:THR:HA | 2.00 | 0.43 |
| 5:CF:558:ASP:O | 5:CF:566:TYR:HE2 | 2.02 | 0.43 |
| 5:CG:328:LEU:HG | 5:CG:329:PHE:H | 1.84 | 0.43 |
| 5:CF:416:ILE:HG23 | 5:CH:472:TYR:HA | 2.00 | 0.43 |
| 5:CH:49:TRP:CZ3 | 5:CH:96:ARG:HD2 | 2.54 | 0.43 |
| 6:CI:90:PHE:O | 6:CI:154:SER:HB2 | 2.19 | 0.43 |
| 6:CI:64:ILE:HG23 | 6:CI:217:ARG:HH12 | 1.84 | 0.43 |
| 6:CJ:64:ILE:HG23 | 6:CJ:217:ARG:HH12 | 1.84 | 0.43 |
| 6:CJ:43:LEU:O | 6:DA:111:GLY:HA3 | 2.18 | 0.43 |
| 3:D:140:GLY:HA2 | 3:D:163:SER:OG | 2.19 | 0.43 |
| 7:DC:146:SER:HB2 | 7:DC:149:GLN:HG2 | 2.01 | 0.43 |
| 7:DC:232:THR:HG22 | 7:DC:235:GLU:HG3 | 2.00 | 0.43 |
| 7:DC:46:GLY:O | 7:DC:47:VAL:HG23 | 2.19 | 0.43 |
| 7:DB:447:HIS:CE1 | 7:DD:445:HIS:CE1 | 3.06 | 0.43 |
| 7:DB:429:CYS:HA | 7:DD:511:GLU:OE1 | 2.19 | 0.43 |
| 8:DE:5:ASP:HA | 8:DE:8:ARG:HB3 | 2.00 | 0.43 |
| 8:DF:15:PHE:N | 8:DF:15:PHE:CD1 | 2.84 | 0.43 |
| 10:DH:286:VAL:HG13 | 14:YF:100[B]:LYS:HE2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:DI:43:TYR:O | 11:DI:44:ARG:HB2 | 2.19 | 0.43 |
| 11:DI:74:LEU:HD12 | 11:DI:74:LEU:HA | 1.78 | 0.43 |
| 1:EA:227:ARG:HH21 | 1:EB:81:ARG:NH2 | 2.17 | 0.43 |
| 1:EA:494:THR:HG22 | 1:EA:498:GLY:HA2 | 2.01 | 0.43 |
| 1:EA:592:ILE:O | 1:EA:608:LYS:HD2 | 2.19 | 0.43 |
| 1:EB:49:GLU:HA | 1:EB:54:ASN:ND2 | 2.28 | 0.43 |
| 2:EC:131:ASN:OD1 | 2:EC:133:ASP:N | 2.50 | 0.43 |
| 2:EC:321:VAL:HA | 2:EC:326:VAL:HA | 2.01 | 0.43 |
| 2:EC:139:ASN:HA | 2:EC:555:ARG:NH2 | 2.34 | 0.43 |
| 2:EC:572:ASN:CB | 2:EC:611:ILE:HG22 | 2.48 | 0.43 |
| 2:EC:613:LYS:HG3 | 2:EC:614:PRO:HD3 | 2.00 | 0.43 |
| 2:EC:669:GLU:O | 2:EC:672:ILE:N | 2.51 | 0.43 |
| 3:ED:279:LEU:HA | 3:ED:279:LEU:HD23 | 1.76 | 0.43 |
| 4:EG:28:GLY:O | 4:EG:32:ASN:ND2 | 2.51 | 0.43 |
| 4:EH:145:LYS:N | 4:EH:165:GLU:O | 2.49 | 0.43 |
| 4:EH:224:ASP:OD2 | 4:EH:227:ASN:HB2 | 2.19 | 0.43 |
| 4:EH:28:GLY:O | 4:EH:32:ASN:ND2 | 2.51 | 0.43 |
| 5:EI:285:LEU:HD11 | 5:EI:375:PHE:CB | 2.41 | 0.43 |
| 5:EI:302:GLU:HG3 | 5:EI:303:PRO:HD2 | 2.00 | 0.43 |
| 5:EI:326:MET:HB2 | 5:EI:326:MET:HE3 | 1.80 | 0.43 |
| 5:EI:326:MET:HG3 | 5:EI:327:PRO:CD | 2.43 | 0.43 |
| 5:EJ:304:ILE:HD11 | 5:EJ:309:LEU:HA | 2.00 | 0.43 |
| 2:EC:221:ALA:N | 5:EJ:562:SER:OG | 2.45 | 0.43 |
| 4:F:209:VAL:HG13 | 4:F:271:GLY:O | 2.19 | 0.43 |
| 5:FA:186:TYR:HB3 | 5:FA:227:GLY:CA | 2.49 | 0.43 |
| 6:FB:130:ARG:O | 6:FB:134:GLN:HG3 | 2.18 | 0.43 |
| 6:FB:10:VAL:CG1 | 6:FD:10:VAL:HG21 | 2.49 | 0.43 |
| 7:FE:32:VAL:HG22 | 7:FE:36:ILE:HG12 | 2.01 | 0.43 |
| 7:FE:520:ASN:ND2 | 7:FF:434:VAL:HG21 | 2.34 | 0.43 |
| 7:FG:110:VAL:HG12 | 7:FG:111:ASN:H | 1.84 | 0.43 |
| 7:FG:493:GLU:HG3 | 7:FG:496:ARG:HH21 | 1.84 | 0.43 |
| 8:FH:88:TRP:CE3 | 8:FH:134:PRO:HD3 | 2.53 | 0.43 |
| 12:DJ:143:TYR:OH | 10:GA:218:ASP:OD2 | 2.24 | 0.43 |
| 1:GD:210:THR:CG2 | 1:GD:226:MET:H | 2.31 | 0.43 |
| 1:GE:371:TYR:HB3 | 1:GE:373:PHE:CE1 | 2.54 | 0.43 |
| 2:EC:603:ARG:HH12 | 1:GE:390:GLU:HG2 | 1.84 | 0.43 |
| 1:GD:227:ARG:HH21 | 1:GE:81:ARG:NH2 | 2.17 | 0.43 |
| 3:GG:150:LYS:HA | 3:GG:160:TRP:CZ3 | 2.53 | 0.43 |
| 3:GG:71:MET:HB2 | 3:GG:71:MET:HE2 | 1.91 | 0.43 |
| 3:GH:191:LEU:HA | 3:GH:191:LEU:HD23 | 1.76 | 0.43 |
| 3:GH:204:THR:O | 3:GH:207:TYR:N | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:GH:228:ASN:HA | 3:GH:229:LEU:HD13 | 2.01 | 0.43 |
| 5:HB:107:VAL:HB | 5:HB:126:ILE:HB | 2.01 | 0.43 |
| 5:HB:185:SER:HB2 | 5:HB:228:PHE:HE1 | 1.84 | 0.43 |
| 5:HD:338:ASP:HB3 | 5:HD:349:TRP:HD1 | 1.78 | 0.43 |
| 6:HE:195:LEU:HD13 | 6:HE:215:PHE:CE1 | 2.52 | 0.43 |
| 6:HF:135:GLU:O | 6:HF:139:SER:N | 2.26 | 0.43 |
| 6:HG:108:LEU:HD23 | 6:HG:113:PRO:HA | 2.00 | 0.43 |
| 6:HE:74:LYS:HG3 | 6:HG:70:ILE:HD11 | 2.00 | 0.43 |
| 7:HH:183:ALA:O | 7:HH:184:THR:HG23 | 2.19 | 0.43 |
| 7:HH:190:VAL:HG23 | 7:HI:188:GLN:HB3 | 2.00 | 0.43 |
| 7:HH:221:THR:HG23 | 7:HH:224:TYR:H | 1.84 | 0.43 |
| 7:HH:227:VAL:HG23 | 7:HI:225:LYS:HD3 | 2.01 | 0.43 |
| 7:HI:77:THR:CG2 | 7:HI:80:THR:H | 2.31 | 0.43 |
| 7:HJ:417:ASN:HB3 | 7:HJ:421:GLY:HA2 | 2.01 | 0.43 |
| 7:HJ:47:VAL:HG12 | 7:HJ:48:PRO:N | 2.34 | 0.43 |
| 5:I:134:GLU:O | 5:I:145:TYR:HA | 2.19 | 0.43 |
| 5:I:22:GLY:O | 5:I:26:ILE:N | 2.37 | 0.43 |
| 10:ID:215:SER:O | 12:IF:191:LEU:HD13 | 2.19 | 0.43 |
| 5:J:180:VAL:HG22 | 5:J:181:PHE:H | 1.84 | 0.43 |
| 5:J:190:ASN:HD22 | 5:J:247:PHE:HD2 | 1.65 | 0.43 |
| 5:J:389:ASP:N | 5:J:389:ASP:OD1 | 2.51 | 0.43 |
| 5:K:177:PHE:CD2 | 5:K:230:ILE:HD11 | 2.48 | 0.43 |
| 6:L:71:ILE:O | 6:L:215:PHE:N | 2.36 | 0.43 |
| 6:M:43:LEU:O | 6:N:111:GLY:HA3 | 2.19 | 0.43 |
| 7:O:183:ALA:O | 7:O:187:ASP:HB2 | 2.19 | 0.43 |
| 7:O:448:ALA:HA | 7:Q:483:PHE:HA | 2.01 | 0.43 |
| 7:Q:20:PRO:CD | 7:Q:29:ILE:HG21 | 2.49 | 0.43 |
| 8:R:134:PRO:HA | 8:R:157:LEU:HD23 | 2.01 | 0.43 |
| 9:T:108:ILE:O | 9:T:121:GLN:HA | 2.19 | 0.43 |
| 11:V:44:ARG:HG2 | 11:V:45:LEU:N | 2.33 | 0.43 |
| 12:W:140:ASP:OD1 | 12:W:141:TRP:N | 2.52 | 0.43 |
| 1:X:192:ILE:HG22 | 1:X:272:TYR:CE1 | 2.54 | 0.43 |
| 1:X:523:VAL:O | 1:X:531:GLU:HB2 | 2.19 | 0.43 |
| 1:Y:206:TRP:CG | 1:Y:222:THR:HB | 2.53 | 0.43 |
| 13:YA:327[D]:VAL:O | 13:YA:331[D]:ILE:HG22 | 2.19 | 0.43 |
| 13:YA:132[C]:LEU:O | 13:YA:390[C]:VAL:HG11 | 2.19 | 0.43 |
| 13:YA:389[E]:TYR:O | 13:YA:405[E]:ASP:HB2 | 2.19 | 0.43 |
| 13:YA:76[A]:PRO:HG3 | 13:YA:96[A]:VAL:CG1 | 2.48 | 0.43 |
| 13:YB:112[A]:GLU:C | 13:YB:115[A]:SER:HB3 | 2.39 | 0.43 |
| 13:YB:219[E]:LYS:HB2 | 13:YB:219[E]:LYS:HE3 | 1.80 | 0.43 |
| 13:YB:454[A]:LYS:C | 13:YB:455[A]:LYS:HG3 | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:454[D]:LYS:C | 13:YB:455[D]:LYS:HG3 | 2.39 | 0.43 |
| 13:YB:458[B]:VAL:HG21 | 13:YC:454[B]:LYS:HD2 | 1.99 | 0.43 |
| 13:YA:471[E]:LEU:O | 13:YB:463[E]:ILE:HA | 2.18 | 0.43 |
| 13:YB:83[C]:TYR:OH | 13:YB:85[C]:HIS:HE1 | 2.02 | 0.43 |
| 13:YC:132[F]:LEU:O | 13:YC:390[F]:VAL:HG11 | 2.19 | 0.43 |
| 13:YC:200[A]:ILE:HD13 | 13:YC:236[A]:ILE:HD12 | 2.01 | 0.43 |
| 13:YC:200[D]:ILE:HD13 | 13:YC:236[D]:ILE:HD12 | 2.01 | 0.43 |
| 13:YC:236[B]:ILE:HG23 | 13:YC:240[B]:GLU:HB2 | 1.99 | 0.43 |
| 13:YC:320[D]:THR:HG22 | 13:YC:323[D]:ARG:HB3 | 2.00 | 0.43 |
| 13:YC:327[A]:VAL:O | 13:YC:331[A]:ILE:HG22 | 2.19 | 0.43 |
| 13:YC:454[A]:LYS:C | 13:YC:455[A]:LYS:HG3 | 2.39 | 0.43 |
| 13:YA:452[C]:GLY:O | 13:YC:460[C]:GLY:N | 2.52 | 0.43 |
| 13:YA:544[F]:TRP:HB2 | 13:YC:552[F]:GLU:HB2 | 2.00 | 0.43 |
| 13:YB:566[D]:THR:HG23 | 13:YC:558[D]:SER:HA | 2.01 | 0.43 |
| 14:YD:75[F]:ALA:HB2 | 14:YD:83[F]:VAL:HA | 2.00 | 0.43 |
| 14:YD:80[E]:ILE:H | 14:YD:80[E]:ILE:HD13 | 1.84 | 0.43 |
| 14:YD:88[E]:TYR:HD1 | 14:YD:110[E]:GLY:C | 2.22 | 0.43 |
| 14:YE:17[D]:PHE:HE2 | 14:YE:26[D]:ASN:HA | 1.84 | 0.43 |
| 14:YF:170[D]:LEU:HD23 | 14:YF:170[D]:LEU:HA | 1.68 | 0.43 |
| 14:YF:17[F]:PHE:HE2 | 14:YF:26[F]:ASN:HA | 1.83 | 0.43 |
| 14:YF:308[E]:ALA:O | 14:YF:357[E]:MET:N | 2.51 | 0.43 |
| 2:Z:724:ALA:C | 2:Z:726:PHE:H | 2.20 | 0.43 |
| 15:ZA:37[D]:LEU:HB2 | 15:ZA:75[D]:VAL:HB | 2.01 | 0.43 |
| 1:A:275:THR:OG1 | 1:A:275:THR:O | 2.36 | 0.43 |
| 1:A:392:ILE:HG23 | 1:A:408:ILE:HD12 | 2.01 | 0.43 |
| 4:AA:190:PRO:HA | 4:AA:262:THR:HA | 2.01 | 0.43 |
| 4:AA:44:ASP:O | 4:AA:59:GLN:NE2 | 2.52 | 0.43 |
| 4:AB:201:LYS:NZ | 4:AB:220:ASN:OD1 | 2.37 | 0.43 |
| 5:AC:355:ASP:OD1 | 5:AC:356:TYR:N | 2.49 | 0.43 |
| 5:AD:328:LEU:HG | 5:AD:329:PHE:H | 1.84 | 0.43 |
| 5:AD:322:GLY:N | 5:AD:360:THR:HG23 | 2.33 | 0.43 |
| 5:AD:98:VAL:HG12 | 5:AD:99:PHE:CD2 | 2.46 | 0.43 |
| 5:AE:363:ASN:HD21 | 7:FG:472:ARG:NE | 2.15 | 0.43 |
| 5:AE:478:TRP:CH2 | 5:AE:600:ARG:HB2 | 2.54 | 0.43 |
| 6:AF:6:ASN:HB3 | 6:AG:12:SER:HB3 | 2.01 | 0.43 |
| 6:AF:198:ALA:O | 6:AG:203:LEU:HB3 | 2.19 | 0.43 |
| 6:AG:73:ASN:ND2 | 6:AG:215:PHE:HE2 | 2.16 | 0.43 |
| 6:AG:43:LEU:HD11 | 6:AH:141:THR:HG22 | 2.00 | 0.43 |
| 7:AI:176:ILE:HG23 | 7:AI:177:ALA:H | 1.84 | 0.43 |
| 7:AI:228:ILE:O | 7:AJ:225:LYS:HA | 2.19 | 0.43 |
| 7:AI:466:SER:HB3 | 7:AI:468:PHE:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:12:GLU:CG | 7:AJ:15:TYR:H | 2.31 | 0.43 |
| 7:AI:227:VAL:HG23 | 7:AJ:225:LYS:HD3 | 2.00 | 0.43 |
| 1:B:508:ARG:HE | 1:B:544:ASP:HB2 | 1.83 | 0.43 |
| 1:B:55:VAL:HG21 | 2:C:657:TYR:CZ | 2.54 | 0.43 |
| 7:AJ:227:VAL:CG2 | 7:BA:225:LYS:HB3 | 2.49 | 0.43 |
| 7:BA:417:ASN:HB3 | 7:BA:421:GLY:HA2 | 2.01 | 0.43 |
| 7:BA:493:GLU:HG3 | 7:BA:496:ARG:HH21 | 1.84 | 0.43 |
| 1:BH:192:ILE:HG22 | 1:BH:272:TYR:CE1 | 2.54 | 0.43 |
| 1:BH:347:THR:O | 1:BH:350:SER:N | 2.52 | 0.43 |
| 1:BH:523:VAL:O | 1:BH:531:GLU:HB2 | 2.18 | 0.43 |
| 1:BI:174:ARG:HA | 1:BI:270:ILE:O | 2.19 | 0.43 |
| 1:BI:429:LEU:O | 1:BI:429:LEU:HD12 | 2.19 | 0.43 |
| 2:BJ:146:LEU:HD12 | 2:BJ:146:LEU:C | 2.39 | 0.43 |
| 2:BJ:194:GLU:HG2 | 2:BJ:199:LEU:HA | 2.01 | 0.43 |
| 2:BJ:228:ARG:HD2 | 5:CH:556:GLN:NE2 | 2.34 | 0.43 |
| 2:BJ:241:SER:O | 2:BJ:244:THR:OG1 | 2.25 | 0.43 |
| 2:BJ:457:ASN:O | 2:BJ:458:ASP:C | 2.57 | 0.43 |
| 1:BI:50:GLY:HA2 | 2:BJ:657:TYR:OH | 2.18 | 0.43 |
| 2:BJ:690:ILE:HA | 2:BJ:690:ILE:HD12 | 1.87 | 0.43 |
| 2:C:314:THR:HG23 | 2:C:317:TYR:HB2 | 2.01 | 0.43 |
| 2:C:58:ASN:HB3 | 4:G:155:ASN:ND2 | 2.33 | 0.43 |
| 2:C:653:MET:SD | 2:C:654:PRO:HD2 | 2.59 | 0.43 |
| 2:BJ:819:ARG:NH2 | 3:CB:215:GLU:OE1 | 2.50 | 0.43 |
| 4:CD:107:VAL:O | 4:CD:148:LEU:N | 2.39 | 0.43 |
| 4:CD:28:GLY:O | 4:CD:32:ASN:ND2 | 2.51 | 0.43 |
| 4:CE:124:ILE:HB | 4:CE:137:LEU:HB3 | 2.01 | 0.43 |
| 5:CF:36:GLU:OE1 | 5:CF:66:LYS:HG2 | 2.19 | 0.43 |
| 5:CG:341:GLU:C | 5:CG:343:SER:H | 2.22 | 0.43 |
| 2:BJ:228:ARG:NH2 | 5:CH:559:PRO:HD3 | 2.34 | 0.43 |
| 5:CH:469:PRO:HD3 | 5:CH:598:TRP:CE2 | 2.53 | 0.43 |
| 5:CH:67:SER:HA | 5:CH:94:ARG:HB2 | 2.01 | 0.43 |
| 6:CI:86:ASP:CG | 6:CI:180:GLN:HE21 | 2.19 | 0.43 |
| 6:CJ:10:VAL:HA | 6:DA:13:ARG:HB2 | 1.99 | 0.43 |
| 2:C:947:VAL:HB | 3:D:119:TYR:HB3 | 2.00 | 0.43 |
| 7:DB:125:LEU:O | 7:DB:129:PHE:N | 2.45 | 0.43 |
| 7:DB:248:ALA:O | 7:DB:252:GLY:N | 2.44 | 0.43 |
| 7:DC:267:THR:O | 7:DC:285:ALA:HA | 2.19 | 0.43 |
| 7:DC:359:TRP:CH2 | 7:DC:524:LYS:HB2 | 2.54 | 0.43 |
| 7:DB:75:ALA:HB1 | 7:DC:75:ALA:HB1 | 2.00 | 0.43 |
| 7:DC:85:LEU:C | 7:DC:88:PRO:HD3 | 2.40 | 0.43 |
| 7:DD:349:TRP:NE1 | 7:DD:351:ALA:HB3 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DD:417:ASN:HB3 | 7:DD:421:GLY:HA2 | 2.01 | 0.43 |
| 12:DJ:5:GLU:O | 12:DJ:9:ASN:N | 2.41 | 0.43 |
| 1:EB:174:ARG:HA | 1:EB:270:ILE:O | 2.19 | 0.43 |
| 1:EB:382:LEU:HA | 1:EB:382:LEU:HD23 | 1.78 | 0.43 |
| 1:EB:485:VAL:HG22 | 1:EB:624:TYR:HD1 | 1.83 | 0.43 |
| 1:EB:654:ASP:OD1 | 1:EB:655:LEU:N | 2.52 | 0.43 |
| 2:EC:300:LEU:N | 2:EC:301:PRO:HD3 | 2.34 | 0.43 |
| 2:EC:494:GLU:HB2 | 2:EC:498:TRP:CB | 2.49 | 0.43 |
| 3:ED:254:ASP:HB3 | 3:ED:257:TYR:HD2 | 1.84 | 0.43 |
| 3:ED:64:SER:OG | 3:ED:67:GLY:N | 2.35 | 0.43 |
| 4:EF:224:ASP:OD2 | 4:EF:227:ASN:HB2 | 2.19 | 0.43 |
| 4:EF:44:ASP:O | 4:EF:59:GLN:NE2 | 2.52 | 0.43 |
| 4:EH:192:PHE:O | 4:EH:261:VAL:N | 2.51 | 0.43 |
| 4:EH:44:ASP:O | 4:EH:59:GLN:NE2 | 2.52 | 0.43 |
| 5:EI:202:TYR:CD1 | 5:EI:225:LEU:HD12 | 2.54 | 0.43 |
| 5:EI:321:ALA:O | 5:EI:324:VAL:HG12 | 2.19 | 0.43 |
| 5:EI:261:ARG:HB2 | 5:EI:383:ILE:HB | 2.01 | 0.43 |
| 5:EI:403:THR:HA | 5:EI:406:LEU:HB2 | 2.01 | 0.43 |
| 5:EJ:102:TRP:N | 5:EJ:102:TRP:CD1 | 2.86 | 0.43 |
| 5:EJ:135:LEU:HA | 5:EJ:144:GLU:O | 2.18 | 0.43 |
| 5:EJ:247:PHE:CZ | 5:FA:162:VAL:HG11 | 2.54 | 0.43 |
| 5:EJ:389:ASP:OD2 | 5:FA:254:TRP:HD1 | 2.01 | 0.43 |
| 5:EJ:421:ASN:HB2 | 5:EJ:434:GLU:CG | 2.49 | 0.43 |
| 5:FA:169:VAL:O | 5:FA:238:ILE:HA | 2.19 | 0.43 |
| 5:FA:176:ASP:HA | 5:FA:231:ARG:HA | 1.99 | 0.43 |
| 5:FA:186:TYR:HB3 | 5:FA:227:GLY:C | 2.40 | 0.43 |
| 5:EI:399:ILE:HD12 | 5:FA:399:ILE:HG12 | 2.01 | 0.43 |
| 6:FB:64:ILE:HG23 | 6:FB:217:ARG:HH12 | 1.84 | 0.43 |
| 5:FA:316:ILE:HD11 | 6:FB:7:LYS:NZ | 2.34 | 0.43 |
| 6:FB:6:ASN:HB3 | 6:FC:12:SER:CB | 2.48 | 0.43 |
| 6:FC:90:PHE:O | 6:FC:154:SER:HB2 | 2.19 | 0.43 |
| 6:FD:108:LEU:HD23 | 6:FD:113:PRO:HA | 2.00 | 0.43 |
| 6:FD:47:PHE:HE2 | 6:FD:51:ASN:HB3 | 1.84 | 0.43 |
| 7:FE:163:LEU:HD23 | 7:FE:167:GLN:HB2 | 2.01 | 0.43 |
| 7:FF:129:PHE:CE2 | 7:FF:141:VAL:HG11 | 2.52 | 0.43 |
| 7:FF:342:PRO:HB2 | 7:FF:378:ARG:HH12 | 1.83 | 0.43 |
| 9:FJ:7:LEU:HD23 | 9:FJ:7:LEU:HA | 1.78 | 0.43 |
| 10:GA:139:SER:HA | 10:GA:203:ARG:HG2 | 2.01 | 0.43 |
| 1:GD:392:ILE:HG23 | 1:GD:408:ILE:HD12 | 2.01 | 0.43 |
| 1:GD:64:THR:HG21 | 2:GF:674:TYR:HE2 | 1.83 | 0.43 |
| 1:GD:7:ASN:N | 1:GD:7:ASN:OD1 | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GE:154:ILE:HG22 | 1:GE:155:ARG:O | 2.19 | 0.43 |
| 1:GE:270:ILE:HG21 | 1:GE:270:ILE:HD13 | 1.79 | 0.43 |
| 1:GE:378:PRO:O | 1:GE:379:LYS:HG2 | 2.19 | 0.43 |
| 1:GE:429:LEU:O | 1:GE:429:LEU:HD12 | 2.19 | 0.43 |
| 1:GE:485:VAL:HG11 | 1:GE:650:TYR:CE1 | 2.53 | 0.43 |
| 3:D:70:ASP:OD2 | 2:GF:450:PHE:HE2 | 2.01 | 0.43 |
| 1:GE:55:VAL:HG21 | 2:GF:657:TYR:CZ | 2.54 | 0.43 |
| 2:GF:937:THR:HA | 2:GF:941:GLU:O | 2.19 | 0.43 |
| 3:GG:115:ASN:HD21 | 3:GG:123:GLU:HB3 | 1.83 | 0.43 |
| 3:GG:254:ASP:HB3 | 3:GG:257:TYR:HD2 | 1.84 | 0.43 |
| 5:HB:166:GLU:HB2 | 5:HD:201:TYR:CD2 | 2.53 | 0.43 |
| 5:HB:202:TYR:CD1 | 5:HB:225:LEU:HD12 | 2.54 | 0.43 |
| 5:HB:403:THR:HA | 5:HB:406:LEU:HB2 | 2.01 | 0.43 |
| 5:HB:469:PRO:HA | 5:HB:472:TYR:CZ | 2.54 | 0.43 |
| 5:HC:136:VAL:HG21 | 5:HD:151:ILE:HD11 | 2.01 | 0.43 |
| 5:HC:267:ASP:H | 5:HC:377:HIS:HB2 | 1.84 | 0.43 |
| 5:HC:288:MET:HE2 | 5:HC:292:PRO:HD3 | 2.01 | 0.43 |
| 5:HC:421:ASN:HB2 | 5:HC:434:GLU:CG | 2.49 | 0.43 |
| 5:HC:460:TYR:HE1 | 5:HD:458:THR:HG23 | 1.84 | 0.43 |
| 5:HC:478:TRP:CH2 | 5:HC:600:ARG:HB2 | 2.54 | 0.43 |
| 5:HD:215:PRO:HB3 | 5:HD:229:ASN:O | 2.19 | 0.43 |
| 5:HD:67:SER:HA | 5:HD:94:ARG:HB2 | 2.01 | 0.43 |
| 6:HG:64:ILE:HG23 | 6:HG:217:ARG:HH12 | 1.84 | 0.43 |
| 7:HH:130:GLU:OE2 | 7:HI:132:ARG:NH1 | 2.39 | 0.43 |
| 7:HH:255:SER:O | 7:HH:278:SER:OG | 2.29 | 0.43 |
| 7:HH:300:LEU:HB3 | 7:HI:302:ILE:HD13 | 2.00 | 0.43 |
| 7:HH:378:ARG:NH1 | 7:HJ:355:PRO:HG3 | 2.34 | 0.43 |
| 7:HH:453:GLU:CD | 7:HH:471:THR:H | 2.18 | 0.43 |
| 7:HH:509:GLY:O | 7:HI:443:SER:HA | 2.18 | 0.43 |
| 7:HH:95:TYR:HD1 | 7:HJ:99:ARG:N | 2.17 | 0.43 |
| 7:HH:162:PRO:CB | 7:HI:150:ALA:HA | 2.47 | 0.43 |
| 7:HI:347:MET:HB2 | 7:HI:347:MET:HE3 | 1.77 | 0.43 |
| 7:HJ:101:SER:OG | 7:HJ:102:THR:N | 2.52 | 0.43 |
| 7:HJ:161:THR:H | 7:HJ:164:LYS:HB2 | 1.83 | 0.43 |
| 7:HH:188:GLN:NE2 | 7:HJ:192:GLN:OE1 | 2.52 | 0.43 |
| 7:HJ:349:TRP:NE1 | 7:HJ:351:ALA:HB3 | 2.34 | 0.43 |
| 7:HJ:489:GLU:CD | 7:HJ:502:LEU:H | 2.22 | 0.43 |
| 7:HH:435:GLY:HA2 | 7:HJ:517:ILE:HD11 | 2.01 | 0.43 |
| 5:I:170:GLU:O | 5:I:171:VAL:HG12 | 2.19 | 0.43 |
| 5:I:202:TYR:CD1 | 5:I:225:LEU:HD12 | 2.54 | 0.43 |
| 5:I:229:ASN:OD1 | 5:I:230:ILE:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:304:ILE:HG21 | 5:I:309:LEU:HD12 | 2.01 | 0.43 |
| 5:I:323:THR:HG21 | 5:I:354:THR:HA | 2.00 | 0.43 |
| 5:I:358:VAL:HG23 | 5:I:371:PHE:HD1 | 1.83 | 0.43 |
| 5:I:535:THR:OG1 | 5:K:576:THR:HB | 2.18 | 0.43 |
| 5:I:64:TRP:CZ2 | 5:I:82:PRO:HB2 | 2.54 | 0.43 |
| 8:IA:134:PRO:HA | 8:IA:157:LEU:HD23 | 2.01 | 0.43 |
| 5:J:258:TYR:CD2 | 5:J:259:THR:N | 2.87 | 0.43 |
| 5:K:102:TRP:CZ3 | 5:K:131:SER:HB2 | 2.54 | 0.43 |
| 5:K:157:SER:O | 5:K:160:SER:OG | 2.28 | 0.43 |
| 5:K:215:PRO:HB3 | 5:K:229:ASN:C | 2.40 | 0.43 |
| 5:K:49:TRP:CZ3 | 5:K:96:ARG:HD2 | 2.54 | 0.43 |
| 6:N:108:LEU:HD23 | 6:N:113:PRO:HA | 2.00 | 0.43 |
| 6:N:90:PHE:O | 6:N:154:SER:HB2 | 2.19 | 0.43 |
| 7:O:111:ASN:ND2 | 7:O:114:SER:HB3 | 2.34 | 0.43 |
| 7:O:111:ASN:CG | 7:O:114:SER:HB3 | 2.38 | 0.43 |
| 7:O:141:VAL:HG23 | 7:P:140:GLY:O | 2.19 | 0.43 |
| 7:O:221:THR:HG23 | 7:O:224:TYR:H | 1.83 | 0.43 |
| 7:O:32:VAL:O | 7:O:36:ILE:HG12 | 2.18 | 0.43 |
| 7:O:39:ILE:HG22 | 7:Q:44:VAL:CG2 | 2.49 | 0.43 |
| 7:P:103:ASN:OD1 | 7:P:120:LYS:HG2 | 2.19 | 0.43 |
| 7:O:228:ILE:O | 7:P:225:LYS:HA | 2.19 | 0.43 |
| 7:O:439:ILE:HG12 | 7:Q:515:TRP:CZ3 | 2.54 | 0.43 |
| 8:R:88:TRP:CE3 | 8:R:134:PRO:HD3 | 2.53 | 0.43 |
| 8:S:98:GLU:OE1 | 8:S:98:GLU:N | 2.48 | 0.43 |
| 9:T:64:ASN:O | 9:T:69:THR:HG21 | 2.19 | 0.43 |
| 12:W:164:MET:HB3 | 12:W:237:THR:HG22 | 2.01 | 0.43 |
| 1:X:12:ARG:O | 2:Z:709:TYR:OH | 2.26 | 0.43 |
| 1:X:146:VAL:HG11 | 1:X:172:ILE:HG12 | 2.01 | 0.43 |
| 1:X:192:ILE:HG22 | 1:X:272:TYR:CD1 | 2.54 | 0.43 |
| 1:X:592:ILE:O | 1:X:608:LYS:HD2 | 2.19 | 0.43 |
| 1:Y:154:ILE:HG22 | 1:Y:155:ARG:O | 2.19 | 0.43 |
| 1:Y:299:ASN:OD1 | 1:Y:300:ILE:N | 2.52 | 0.43 |
| 1:Y:330:THR:HG23 | 1:Y:333:ARG:HE | 1.83 | 0.43 |
| 1:Y:524:VAL:HG13 | 1:Y:529:GLY:O | 2.19 | 0.43 |
| 13:YA:112[A]:GLU:C | 13:YA:115[A]:SER:HB3 | 2.39 | 0.43 |
| 13:YA:147[F]:ILE:O | 13:YA:151[F]:ASN:ND2 | 2.47 | 0.43 |
| 13:YA:330[A]:ILE:HD12 | 13:YA:336[A]:LEU:HD12 | 2.01 | 0.43 |
| 13:YA:363[C]:PRO:HB2 | 13:YC:284[C]:MET:HE3 | 2.01 | 0.43 |
| 13:YA:36[B]:PRO:HB2 | 13:YA:38[B]:GLN:OE1 | 2.18 | 0.43 |
| 13:YA:47[A]:ILE:HG23 | 14:YD:123[A]:PRO:CG | 2.47 | 0.43 |
| 13:YA:569[A]:GLY:HA2 | 13:YB:561[A]:SER:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:569[D]:GLY:HA2 | 13:YB:561[D]:SER:O | 2.18 | 0.43 |
| 13:YA:83[B]:TYR:OH | 13:YA:85[B]:HIS:HE1 | 2.02 | 0.43 |
| 13:YB:127[B]:ASN:ND2 | 13:YB:129[B]:THR:OG1 | 2.52 | 0.43 |
| 13:YB:131[D]:VAL:O | 13:YB:134[D]:GLN:N | 2.46 | 0.43 |
| 13:YB:147[B]:ILE:HD11 | 13:YB:188[B]:LEU:HG | 2.00 | 0.43 |
| 13:YB:26[F]:ARG:HD3 | 14:YE:259[F]:LEU:CD2 | 2.48 | 0.43 |
| 13:YB:320[A]:THR:HG22 | 13:YB:323[A]:ARG:HB3 | 2.00 | 0.43 |
| 13:YB:327[A]:VAL:O | 13:YB:331[A]:ILE:HG22 | 2.19 | 0.43 |
| 13:YB:330[F]:ILE:HD12 | 13:YB:336[F]:LEU:HD12 | 2.00 | 0.43 |
| 13:YB:327[D]:VAL:O | 13:YB:331[D]:ILE:HG22 | 2.19 | 0.43 |
| 13:YB:330[D]:ILE:HD12 | 13:YB:336[D]:LEU:HD12 | 2.01 | 0.43 |
| 13:YB:389[B]:TYR:O | 13:YB:405[B]:ASP:HB2 | 2.19 | 0.43 |
| 13:YA:551[C]:THR:O | 13:YB:543[C]:ASP:HA | 2.19 | 0.43 |
| 13:YB:546[F]:VAL:HG11 | 13:YC:542[F]:VAL:HG13 | 2.01 | 0.43 |
| 13:YB:552[E]:GLU:CG | 13:YB:554[E]:MET:HE1 | 2.49 | 0.43 |
| 13:YB:564[D]:GLN:HG3 | 13:YB:566[D]:THR:HG22 | 2.01 | 0.43 |
| 13:YB:66[B]:MET:HA | 13:YB:66[B]:MET:HE3 | 2.00 | 0.43 |
| 13:YC:147[B]:ILE:O | 13:YC:151[B]:ASN:ND2 | 2.47 | 0.43 |
| 13:YC:195[D]:GLU:HG2 | 13:YC:197[D]:TYR:CE2 | 2.54 | 0.43 |
| 13:YC:200[B]:ILE:HD13 | 13:YC:236[B]:ILE:HD12 | 2.01 | 0.43 |
| 13:YC:24[C]:LEU:HA | 13:YC:24[C]:LEU:HD12 | 1.63 | 0.43 |
| 13:YC:280[B]:MET:O | 13:YC:284[B]:MET:HG2 | 2.19 | 0.43 |
| 13:YC:132[D]:LEU:O | 13:YC:390[D]:VAL:HG11 | 2.19 | 0.43 |
| 13:YC:439[C]:TYR:HB3 | 13:YC:441[C]:ILE:CD1 | 2.49 | 0.43 |
| 13:YB:530[B]:VAL:HG22 | 13:YC:522[B]:VAL:HG13 | 2.01 | 0.43 |
| 13:YB:546[D]:VAL:HG11 | 13:YC:542[D]:VAL:HG13 | 2.01 | 0.43 |
| 13:YC:564[B]:GLN:HG3 | 13:YC:566[B]:THR:HG22 | 2.01 | 0.43 |
| 13:YC:66[F]:MET:HE3 | 13:YC:66[F]:MET:HA | 2.00 | 0.43 |
| 13:YA:9[B]:ASN:ND2 | 13:YC:7[B]:ASN:OD1 | 2.52 | 0.43 |
| 13:YC:83[C]:TYR:OH | 13:YC:85[C]:HIS:HE1 | 2.02 | 0.43 |
| 14:YD:132[E]:ILE:HD12 | 14:YD:197[E]:MET:SD | 2.58 | 0.43 |
| 14:YD:330[F]:LYS:HG2 | 14:YE:101[F]:GLY:HA3 | 2.01 | 0.43 |
| 14:YE:114[F]:SER:HA | 14:YE:167[F]:GLU:OE1 | 2.19 | 0.43 |
| 10:DH:285:LEU:HA | 14:YE:215[B]:GLU:HG3 | 2.01 | 0.43 |
| 11:GB:175:SER:HA | 14:YE:217[C]:SER:HB2 | 2.00 | 0.43 |
| 14:YE:364[B]:LEU:HD22 | 14:YE:364[B]:LEU:HA | 1.79 | 0.43 |
| 14:YF:127[F]:ASP:CG | 14:YF:130[F]:GLU:H | 2.20 | 0.43 |
| 11:V:178:ASN:HB3 | 14:YF:217[C]:SER:H | 1.83 | 0.43 |
| 14:YF:308[C]:ALA:O | 14:YF:357[C]:MET:N | 2.52 | 0.43 |
| 2:Z:515:ASN:OD1 | 2:Z:524:CYS:HB3 | 2.17 | 0.43 |
| 2:Z:653:MET:SD | 2:Z:654:PRO:HD2 | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:750:VAL:HG23 | 2:Z:751:LEU:H | 1.84 | 0.43 |
| 2:Z:798:ILE:HG12 | 2:Z:811:VAL:HG12 | 2.00 | 0.43 |
| 15:ZA:37[F]:LEU:HB2 | 15:ZA:75[F]:VAL:HB | 2.01 | 0.43 |
| 1:A:347:THR:O | 1:A:350:SER:N | 2.52 | 0.42 |
| 1:A:561:GLY:H | 1:A:588:LYS:NZ | 2.16 | 0.42 |
| 4:AB:124:ILE:HB | 4:AB:137:LEU:HB3 | 2.01 | 0.42 |
| 5:AC:134:GLU:O | 5:AC:145:TYR:HA | 2.19 | 0.42 |
| 5:AC:322:GLY:HA2 | 5:AC:360:THR:N | 2.34 | 0.42 |
| 5:AE:169:VAL:O | 5:AE:238:ILE:HA | 2.19 | 0.42 |
| 5:AE:338:ASP:HB3 | 5:AE:349:TRP:HD1 | 1.78 | 0.42 |
| 5:AE:67:SER:HA | 5:AE:94:ARG:HB2 | 2.01 | 0.42 |
| 6:AG:130:ARG:O | 6:AG:134:GLN:HG3 | 2.18 | 0.42 |
| 6:AH:217:ARG:HE | 6:AH:219:ALA:C | 2.23 | 0.42 |
| 7:AI:163:LEU:HD23 | 7:AI:167:GLN:HB2 | 2.01 | 0.42 |
| 7:AI:32:VAL:HG22 | 7:AI:36:ILE:HG12 | 2.01 | 0.42 |
| 7:AJ:103:ASN:OD1 | 7:AJ:120:LYS:HG2 | 2.19 | 0.42 |
| 1:B:122:TYR:HB3 | 1:B:152:ILE:HD11 | 2.01 | 0.42 |
| 1:B:154:ILE:HG22 | 1:B:155:ARG:O | 2.19 | 0.42 |
| 1:B:654:ASP:OD1 | 1:B:655:LEU:N | 2.52 | 0.42 |
| 7:AI:19:ASP:HB3 | 7:BA:33:GLN:OE1 | 2.19 | 0.42 |
| 10:BE:139:SER:HA | 10:BE:203:ARG:HG2 | 2.01 | 0.42 |
| 11:BF:31:ASN:O | 11:BF:32:TYR:HB2 | 2.18 | 0.42 |
| 1:BH:157:LYS:O | 1:BH:158:ASN:CG | 2.57 | 0.42 |
| 1:BI:229:THR:OG1 | 1:BI:233:ASN:OD1 | 2.34 | 0.42 |
| 1:BI:348:PHE:HZ | 1:BI:399:TYR:HD2 | 1.65 | 0.42 |
| 1:BI:524:VAL:HG13 | 1:BI:529:GLY:O | 2.19 | 0.42 |
| 1:BI:539:ARG:O | 1:BI:541:VAL:HG23 | 2.19 | 0.42 |
| 1:BI:654:ASP:OD1 | 1:BI:655:LEU:N | 2.52 | 0.42 |
| 2:BJ:246:TYR:HE1 | 2:BJ:255:TYR:CD1 | 2.35 | 0.42 |
| 2:BJ:29:GLY:HA2 | 3:CB:60:TYR:HB3 | 2.01 | 0.42 |
| 2:BJ:145:ALA:O | 2:BJ:586:LEU:HB3 | 2.18 | 0.42 |
| 1:BI:568:ASN:HD21 | 2:BJ:806:LYS:HA | 1.83 | 0.42 |
| 2:C:416:VAL:HG23 | 2:C:417:PHE:H | 1.84 | 0.42 |
| 3:CA:86:LEU:HD23 | 3:CA:86:LEU:HA | 1.68 | 0.42 |
| 4:CD:224:ASP:OD2 | 4:CD:227:ASN:HB2 | 2.19 | 0.42 |
| 4:CE:224:ASP:OD2 | 4:CE:227:ASN:HB2 | 2.19 | 0.42 |
| 5:CF:107:VAL:HB | 5:CF:126:ILE:HB | 2.01 | 0.42 |
| 5:CF:229:ASN:OD1 | 5:CF:230:ILE:N | 2.51 | 0.42 |
| 5:CF:358:VAL:HG23 | 5:CF:371:PHE:HD1 | 1.83 | 0.42 |
| 5:CF:261:ARG:HB2 | 5:CF:383:ILE:HB | 2.01 | 0.42 |
| 5:CG:261:ARG:N | 5:CG:383:ILE:O | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:34:TYR:OH | 5:CG:41:ASP:C | 2.58 | 0.42 |
| 5:CH:320:LEU:HG | 5:CH:357:SER:CB | 2.49 | 0.42 |
| 5:CH:71:ASN:ND2 | 5:CH:73:SER:OG | 2.52 | 0.42 |
| 5:CH:79:ILE:HD12 | 5:CH:81:LEU:HD11 | 2.01 | 0.42 |
| 6:CI:195:LEU:HD13 | 6:CI:215:PHE:CE1 | 2.53 | 0.42 |
| 6:CI:217:ARG:HE | 6:CI:219:ALA:C | 2.23 | 0.42 |
| 7:DB:32:VAL:HG22 | 7:DB:36:ILE:HG12 | 2.01 | 0.42 |
| 7:DB:363:HIS:CD2 | 7:DB:396:ARG:HD3 | 2.54 | 0.42 |
| 7:DC:424:ARG:O | 7:DD:504:ARG:NH2 | 2.35 | 0.42 |
| 7:DD:14:ARG:HG2 | 7:DD:33:GLN:HG2 | 2.01 | 0.42 |
| 7:DB:492:PRO:HD2 | 7:DD:464:ARG:NH2 | 2.33 | 0.42 |
| 8:DF:5:ASP:HA | 8:DF:8:ARG:HB3 | 2.00 | 0.42 |
| 12:DJ:18:ARG:HB2 | 12:DJ:21:MET:HG2 | 2.01 | 0.42 |
| 1:EA:157:LYS:O | 1:EA:158:ASN:CG | 2.57 | 0.42 |
| 1:EA:210:THR:CG2 | 1:EA:226:MET:H | 2.31 | 0.42 |
| 1:EA:347:THR:O | 1:EA:351:GLU:N | 2.43 | 0.42 |
| 1:EA:655:LEU:HD12 | 1:EA:655:LEU:O | 2.19 | 0.42 |
| 2:EC:146:LEU:C | 2:EC:146:LEU:HD12 | 2.39 | 0.42 |
| 2:EC:186:ASP:HB3 | 2:EC:189:ARG:CD | 2.49 | 0.42 |
| 2:EC:18:ALA:HB2 | 2:EC:103:PHE:O | 2.19 | 0.42 |
| 2:EC:341:LEU:HD23 | 2:EC:341:LEU:HA | 1.84 | 0.42 |
| 2:EC:135:VAL:HG12 | 2:EC:589:LYS:HE3 | 2.00 | 0.42 |
| 4:EF:166:SER:OG | 4:EH:173:SER:N | 2.36 | 0.42 |
| 4:EH:190:PRO:HA | 4:EH:262:THR:HA | 2.01 | 0.42 |
| 5:EI:275:SER:OG | 5:EI:281:TYR:HA | 2.18 | 0.42 |
| 5:EI:265:LEU:HD22 | 5:EI:281:TYR:HD2 | 1.84 | 0.42 |
| 5:EI:317:LEU:HD13 | 5:EJ:312:ARG:HH12 | 1.83 | 0.42 |
| 5:EI:319:GLU:HG3 | 5:EJ:262:GLN:OE1 | 2.19 | 0.42 |
| 5:EI:358:VAL:HG23 | 5:EI:371:PHE:HD1 | 1.83 | 0.42 |
| 5:FA:117:ILE:HG13 | 5:FA:118:LYS:H | 1.84 | 0.42 |
| 5:FA:151:ILE:HG23 | 5:FA:152:ASP:N | 2.34 | 0.42 |
| 5:FA:180:VAL:HG22 | 5:FA:181:PHE:H | 1.84 | 0.42 |
| 5:FA:478:TRP:CH2 | 5:FA:600:ARG:HB2 | 2.54 | 0.42 |
| 5:FA:67:SER:HA | 5:FA:94:ARG:HB2 | 2.01 | 0.42 |
| 6:FB:90:PHE:O | 6:FB:154:SER:HB2 | 2.19 | 0.42 |
| 6:FC:82:VAL:HG23 | 6:FC:187:LYS:HE3 | 2.01 | 0.42 |
| 7:FE:185:GLU:HA | 7:FG:193:LEU:HB2 | 2.01 | 0.42 |
| 7:FE:183:ALA:O | 7:FE:187:ASP:HB2 | 2.19 | 0.42 |
| 7:FE:448:ALA:HA | 7:FG:483:PHE:HA | 2.01 | 0.42 |
| 7:FE:503:ASN:ND2 | 7:FG:446:LYS:H | 2.17 | 0.42 |
| 7:FF:491:ASP:HB2 | 7:FF:496:ARG:HG2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FF:359:TRP:CH2 | 7:FF:524:LYS:HB2 | 2.54 | 0.42 |
| 7:FG:14:ARG:HG2 | 7:FG:33:GLN:HG2 | 2.01 | 0.42 |
| 8:FH:25:ILE:O | 8:FH:26:SER:HB3 | 2.19 | 0.42 |
| 9:FJ:108:ILE:O | 9:FJ:121:GLN:HA | 2.19 | 0.42 |
| 4:G:124:ILE:HB | 4:G:137:LEU:HB3 | 2.01 | 0.42 |
| 1:GD:123:ILE:HD11 | 1:GD:295:ILE:HD11 | 2.00 | 0.42 |
| 1:GD:192:ILE:HG22 | 1:GD:272:TYR:CD1 | 2.54 | 0.42 |
| 1:GD:446:ARG:NE | 1:GD:450:GLU:OE2 | 2.51 | 0.42 |
| 1:GD:559:ALA:N | 1:GD:586:ARG:HD2 | 2.33 | 0.42 |
| 1:GE:348:PHE:HZ | 1:GE:399:TYR:HD2 | 1.65 | 0.42 |
| 1:GE:524:VAL:HG13 | 1:GE:529:GLY:O | 2.19 | 0.42 |
| 2:GF:139:ASN:HA | 2:GF:555:ARG:NH2 | 2.34 | 0.42 |
| 2:GF:9:THR:OG1 | 2:GF:10:SER:N | 2.51 | 0.42 |
| 4:GI:209:VAL:HG13 | 4:GI:271:GLY:O | 2.19 | 0.42 |
| 4:GJ:173:SER:N | 4:HA:166:SER:OG | 2.38 | 0.42 |
| 5:HB:460:TYR:CE1 | 5:HC:458:THR:HG23 | 2.54 | 0.42 |
| 5:HD:117:ILE:HG13 | 5:HD:118:LYS:H | 1.84 | 0.42 |
| 5:HD:186:TYR:HB3 | 5:HD:227:GLY:CA | 2.49 | 0.42 |
| 5:HD:290:SER:HB3 | 5:HD:370:HIS:HA | 2.01 | 0.42 |
| 5:HD:478:TRP:CH2 | 5:HD:600:ARG:HB2 | 2.54 | 0.42 |
| 5:HB:318:GLN:NE2 | 6:HG:7:LYS:HB3 | 2.34 | 0.42 |
| 7:HH:139:ASN:N | 7:HJ:143:LYS:HG2 | 2.34 | 0.42 |
| 7:HI:228:ILE:O | 7:HJ:226:GLY:N | 2.49 | 0.42 |
| 7:HI:342:PRO:HB2 | 7:HI:378:ARG:HH12 | 1.83 | 0.42 |
| 7:HI:354:LEU:HD21 | 7:HI:522:ILE:HG21 | 2.00 | 0.42 |
| 7:HI:480:ARG:HD3 | 7:HJ:462:ASN:ND2 | 2.34 | 0.42 |
| 7:HH:464:ARG:NH2 | 7:HI:492:PRO:HD2 | 2.34 | 0.42 |
| 7:HJ:110:VAL:HG12 | 7:HJ:111:ASN:H | 1.84 | 0.42 |
| 7:HH:447:HIS:CE1 | 7:HJ:445:HIS:CE1 | 3.07 | 0.42 |
| 5:I:248:MET:HB2 | 5:I:254:TRP:CD1 | 2.52 | 0.42 |
| 5:I:275:SER:OG | 5:I:281:TYR:HA | 2.18 | 0.42 |
| 5:I:321:ALA:O | 5:I:324:VAL:HG12 | 2.19 | 0.42 |
| 5:I:384:THR:O | 5:I:385:TRP:HD1 | 2.01 | 0.42 |
| 5:I:403:THR:HA | 5:I:406:LEU:HB2 | 2.01 | 0.42 |
| 5:I:49:TRP:HZ3 | 5:I:96:ARG:HD2 | 1.80 | 0.42 |
| 9:IC:10:ASP:OD1 | 9:IC:11:ILE:HG22 | 2.18 | 0.42 |
| 1:GD:46:TYR:HE1 | 9:IC:17:MET:HB2 | 1.83 | 0.42 |
| 10:ID:139:SER:HA | 10:ID:203:ARG:HG2 | 2.01 | 0.42 |
| 12:IF:191:LEU:HA | 12:IF:191:LEU:HD23 | 1.82 | 0.42 |
| 12:IF:99:SER:HB3 | 12:IF:102:GLY:H | 1.84 | 0.42 |
| 5:J:304:ILE:HD11 | 5:J:309:LEU:HA | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:34:TYR:OH | 5:J:41:ASP:C | 2.58 | 0.42 |
| 5:J:421:ASN:HB2 | 5:J:434:GLU:CG | 2.49 | 0.42 |
| 6:M:90:PHE:O | 6:M:154:SER:HB2 | 2.19 | 0.42 |
| 7:O:234:SER:HA | 5:HB:347:GLY:N | 2.34 | 0.42 |
| 7:O:378:ARG:NH1 | 7:Q:355:PRO:HG3 | 2.34 | 0.42 |
| 7:O:300:LEU:HB3 | 7:P:302:ILE:HD13 | 2.00 | 0.42 |
| 7:P:40:SER:HB3 | 7:Q:24:ASN:CB | 2.47 | 0.42 |
| 7:Q:14:ARG:HG2 | 7:Q:33:GLN:HG2 | 2.01 | 0.42 |
| 7:Q:218:SER:O | 7:Q:227:VAL:HG22 | 2.19 | 0.42 |
| 7:Q:417:ASN:HB3 | 7:Q:421:GLY:HA2 | 2.01 | 0.42 |
| 8:S:134:PRO:HA | 8:S:157:LEU:HD23 | 2.01 | 0.42 |
| 1:X:227:ARG:HH21 | 1:Y:81:ARG:NH2 | 2.17 | 0.42 |
| 1:X:328:LEU:HA | 1:X:328:LEU:HD23 | 1.71 | 0.42 |
| 1:X:384:LEU:HA | 1:X:384:LEU:HD23 | 1.83 | 0.42 |
| 1:X:38:ASN:N | 1:X:48:PHE:HE2 | 2.17 | 0.42 |
| 1:X:79:PHE:CE1 | 2:Z:702:GLU:HG2 | 2.53 | 0.42 |
| 1:Y:116:ASP:HB2 | 1:Y:161:TYR:HE2 | 1.84 | 0.42 |
| 1:Y:229:THR:OG1 | 1:Y:233:ASN:OD1 | 2.34 | 0.42 |
| 13:YA:280[D]:MET:O | 13:YA:284[D]:MET:HG2 | 2.19 | 0.42 |
| 13:YA:327[A]:VAL:O | 13:YA:331[A]:ILE:HG22 | 2.19 | 0.42 |
| 13:YA:336[E]:LEU:HA | 13:YA:336[E]:LEU:HD12 | 1.85 | 0.42 |
| 13:YA:132[D]:LEU:O | 13:YA:390[D]:VAL:HG11 | 2.19 | 0.42 |
| 13:YA:439[A]:TYR:HB3 | 13:YA:441[A]:ILE:CD1 | 2.50 | 0.42 |
| 13:YA:552[C]:GLU:CG | 13:YA:554[C]:MET:HE1 | 2.49 | 0.42 |
| 13:YB:154[D]:THR:H | 13:YB:182[D]:ARG:NH2 | 2.17 | 0.42 |
| 13:YB:195[A]:GLU:HG2 | 13:YB:197[A]:TYR:CE2 | 2.54 | 0.42 |
| 13:YB:195[B]:GLU:HG2 | 13:YB:197[B]:TYR:CE2 | 2.54 | 0.42 |
| 13:YB:34[A]:LEU:HD13 | 14:YE:163[A]:THR:CG2 | 2.48 | 0.42 |
| 13:YB:132[A]:LEU:O | 13:YB:390[A]:VAL:HG11 | 2.19 | 0.42 |
| 13:YB:132[E]:LEU:O | 13:YB:390[E]:VAL:HG11 | 2.19 | 0.42 |
| 13:YB:442[E]:THR:HB | 13:YC:434[E]:THR:HB | 2.01 | 0.42 |
| 13:YA:471[F]:LEU:O | 13:YB:463[F]:ILE:HA | 2.18 | 0.42 |
| 13:YB:530[E]:VAL:HG22 | 13:YC:522[E]:VAL:HG13 | 2.01 | 0.42 |
| 13:YB:534[C]:LEU:HD11 | 13:YB:536[C]:TRP:NE1 | 2.32 | 0.42 |
| 13:YA:560[B]:ILE:O | 13:YB:553[B]:LYS:HA | 2.18 | 0.42 |
| 13:YA:61[E]:ILE:HA | 13:YB:76[E]:PRO:HB2 | 2.00 | 0.42 |
| 13:YC:195[F]:GLU:HG2 | 13:YC:197[F]:TYR:CE2 | 2.55 | 0.42 |
| 13:YC:277[E]:LEU:HA | 13:YC:277[E]:LEU:HD23 | 1.79 | 0.42 |
| 13:YC:280[A]:MET:O | 13:YC:284[A]:MET:HG2 | 2.19 | 0.42 |
| 13:YC:280[D]:MET:O | 13:YC:284[D]:MET:HG2 | 2.19 | 0.42 |
| 13:YC:320[A]:THR:HG22 | 13:YC:323[A]:ARG:HB3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:330[E]:ILE:HD12 | 13:YC:336[E]:LEU:HD12 | 2.01 | 0.42 |
| 13:YA:9[A]:ASN:ND2 | 13:YC:7[A]:ASN:OD1 | 2.51 | 0.42 |
| 14:YD:112[D]:ILE:HB | 14:YD:140[D]:TYR:OH | 2.19 | 0.42 |
| 14:YD:43[E]:SER:O | 14:YD:189[E]:TRP:HB2 | 2.19 | 0.42 |
| 14:YD:75[B]:ALA:HB2 | 14:YD:83[B]:VAL:HA | 2.01 | 0.42 |
| 14:YE:112[F]:ILE:HB | 14:YE:140[F]:TYR:OH | 2.19 | 0.42 |
| 14:YE:172[C]:TYR:CZ | 14:YE:176[C]:VAL:HG21 | 2.54 | 0.42 |
| 10:ID:286:VAL:H | 14:YE:215[D]:GLU:CD | 2.23 | 0.42 |
| 14:YD:242[E]:PRO:HD2 | 14:YE:91[E]:LYS:O | 2.19 | 0.42 |
| 14:YF:172[F]:TYR:CZ | 14:YF:176[F]:VAL:HG21 | 2.54 | 0.42 |
| 14:YF:86[B]:ARG:HD2 | 14:YF:192[B]:ILE:HD12 | 2.01 | 0.42 |
| 2:Z:725:ARG:HA | 2:Z:728:GLU:HB3 | 2.00 | 0.42 |
| 2:Z:761:GLU:HB2 | 2:Z:862:TYR:CE1 | 2.54 | 0.42 |
| 1:A:592:ILE:O | 1:A:608:LYS:HD2 | 2.19 | 0.42 |
| 4:AA:100:ARG:NH2 | 4:AA:128:ASP:OD1 | 2.53 | 0.42 |
| 4:AA:124:ILE:HB | 4:AA:137:LEU:HB3 | 2.01 | 0.42 |
| 4:AA:224:ASP:OD2 | 4:AA:227:ASN:HB2 | 2.19 | 0.42 |
| 4:AA:240:VAL:HG22 | 4:AB:231:ILE:HD13 | 2.01 | 0.42 |
| 5:AC:323:THR:CG2 | 5:AC:359:GLU:HB2 | 2.48 | 0.42 |
| 5:AE:102:TRP:CZ3 | 5:AE:131:SER:HB2 | 2.53 | 0.42 |
| 5:AE:155:THR:O | 5:AE:156:SER:OG | 2.32 | 0.42 |
| 6:AF:164:GLN:HE22 | 6:AH:54:SER:HA | 1.83 | 0.42 |
| 6:AF:217:ARG:HE | 6:AF:219:ALA:C | 2.23 | 0.42 |
| 7:AI:221:THR:HG23 | 7:AI:224:TYR:H | 1.83 | 0.42 |
| 7:AI:363:HIS:CD2 | 7:AI:396:ARG:HD3 | 2.54 | 0.42 |
| 7:AJ:146:SER:HB2 | 7:AJ:149:GLN:HG2 | 2.01 | 0.42 |
| 7:AJ:190:VAL:HG12 | 7:BA:190:VAL:HG13 | 2.02 | 0.42 |
| 7:AJ:85:LEU:C | 7:AJ:88:PRO:HD3 | 2.40 | 0.42 |
| 1:B:330:THR:HG23 | 1:B:333:ARG:HE | 1.83 | 0.42 |
| 1:B:52:ARG:HD3 | 2:C:657:TYR:CD1 | 2.52 | 0.42 |
| 1:B:610:ASN:ND2 | 2:C:804:ASN:HA | 2.33 | 0.42 |
| 7:BA:349:TRP:NE1 | 7:BA:351:ALA:HB3 | 2.34 | 0.42 |
| 7:AJ:515:TRP:CE3 | 7:BA:439:ILE:HA | 2.55 | 0.42 |
| 7:BA:58:LEU:HD21 | 7:BA:75:ALA:H | 1.84 | 0.42 |
| 8:BB:15:PHE:CD1 | 8:BB:15:PHE:N | 2.84 | 0.42 |
| 10:BE:338:LEU:HD23 | 10:BE:338:LEU:HA | 1.86 | 0.42 |
| 11:BF:178:ASN:H | 14:YE:217[A]:SER:C | 2.21 | 0.42 |
| 1:BH:178:ILE:HD12 | 1:BH:178:ILE:HA | 1.84 | 0.42 |
| 1:BH:306:ASP:OD1 | 1:BH:306:ASP:N | 2.52 | 0.42 |
| 1:BI:167:LEU:HA | 1:BI:167:LEU:HD23 | 1.85 | 0.42 |
| 1:BI:199:LEU:HD21 | 1:BI:224:TYR:CG | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:371:TYR:HB3 | 1:BI:373:PHE:CE1 | 2.54 | 0.42 |
| 2:BJ:300:LEU:N | 2:BJ:301:PRO:HD3 | 2.34 | 0.42 |
| 2:BJ:726:PHE:O | 2:BJ:729:SER:OG | 2.16 | 0.42 |
| 2:C:18:ALA:HB2 | 2:C:103:PHE:O | 2.19 | 0.42 |
| 2:C:222:VAL:HG12 | 2:C:224:LEU:HB2 | 2.01 | 0.42 |
| 2:C:439:LYS:HG3 | 2:C:440:LEU:HD12 | 2.02 | 0.42 |
| 2:C:480:LEU:CD2 | 2:C:488:MET:HB2 | 2.49 | 0.42 |
| 2:C:613:LYS:HG3 | 2:C:614:PRO:HD3 | 2.00 | 0.42 |
| 2:C:690:ILE:HA | 2:C:690:ILE:HD12 | 1.87 | 0.42 |
| 3:CA:197:ASP:OD1 | 3:CA:198:VAL:N | 2.45 | 0.42 |
| 3:CA:16:PHE:HB2 | 3:CB:310:ILE:HB | 2.00 | 0.42 |
| 5:CF:181:PHE:HE2 | 5:CF:246:THR:HG22 | 1.83 | 0.42 |
| 5:CF:323:THR:CG2 | 5:CF:354:THR:HG23 | 2.48 | 0.42 |
| 5:CF:336:SER:HB3 | 5:CF:348:THR:O | 2.20 | 0.42 |
| 5:CF:403:THR:HA | 5:CF:406:LEU:HB2 | 2.01 | 0.42 |
| 5:CG:129:ARG:HG3 | 5:CG:130:PHE:N | 2.33 | 0.42 |
| 5:CG:250:GLY:N | 5:CH:158:ASP:HB3 | 2.35 | 0.42 |
| 5:CG:285:LEU:HD21 | 5:CG:375:PHE:N | 2.21 | 0.42 |
| 5:CG:483:GLN:O | 5:CG:485:LYS:HG2 | 2.20 | 0.42 |
| 5:CH:186:TYR:HB3 | 5:CH:227:GLY:CA | 2.49 | 0.42 |
| 5:CH:215:PRO:HB3 | 5:CH:229:ASN:O | 2.19 | 0.42 |
| 5:CH:299:ILE:HA | 5:CH:300:PRO:HD3 | 1.89 | 0.42 |
| 5:CH:357:SER:HA | 5:CH:371:PHE:CD1 | 2.54 | 0.42 |
| 6:CJ:90:PHE:O | 6:CJ:154:SER:HB2 | 2.19 | 0.42 |
| 6:DA:90:PHE:O | 6:DA:154:SER:HB2 | 2.19 | 0.42 |
| 5:CF:318:GLN:NE2 | 6:DA:4:LEU:O | 2.49 | 0.42 |
| 7:DB:111:ASN:ND2 | 7:DB:114:SER:HB3 | 2.34 | 0.42 |
| 7:DB:276:ASP:OD1 | 7:DC:260:ARG:NH2 | 2.49 | 0.42 |
| 7:DB:408:HIS:CE1 | 7:DD:437:VAL:HG21 | 2.53 | 0.42 |
| 7:DD:20:PRO:CD | 7:DD:29:ILE:HG21 | 2.49 | 0.42 |
| 8:DE:130:LYS:NZ | 8:DE:163:GLU:OE2 | 2.36 | 0.42 |
| 12:DJ:99:SER:HB3 | 12:DJ:102:GLY:H | 1.84 | 0.42 |
| 12:DJ:221:ILE:HA | 12:DJ:221:ILE:HD12 | 1.80 | 0.42 |
| 1:EA:337:GLN:O | 1:EA:348:PHE:HZ | 2.02 | 0.42 |
| 1:EB:206:TRP:CG | 1:EB:222:THR:HB | 2.53 | 0.42 |
| 2:EC:1005:ARG:HG2 | 2:EC:1006:ASP:O | 2.19 | 0.42 |
| 2:EC:416:VAL:HG23 | 2:EC:417:PHE:H | 1.84 | 0.42 |
| 2:EC:548:ILE:HG21 | 2:EC:555:ARG:H | 1.84 | 0.42 |
| 2:EC:927:THR:HB | 2:EC:987:ARG:HA | 2.00 | 0.42 |
| 2:EC:937:THR:HA | 2:EC:941:GLU:O | 2.19 | 0.42 |
| 2:EC:9:THR:OG1 | 2:EC:10:SER:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:ED:140:GLY:HA2 | 3:ED:163:SER:OG | 2.19 | 0.42 |
| 3:ED:294:LYS:N | 3:ED:297:TYR:OH | 2.42 | 0.42 |
| 2:EC:819:ARG:NH2 | 3:EE:215:GLU:OE1 | 2.50 | 0.42 |
| 2:BJ:483:LYS:HZ3 | 3:EE:228:ASN:HB2 | 1.84 | 0.42 |
| 4:EF:145:LYS:N | 4:EF:165:GLU:O | 2.49 | 0.42 |
| 5:EI:184:THR:H | 5:EI:307:ASN:ND2 | 2.13 | 0.42 |
| 5:EI:336:SER:HB3 | 5:EI:348:THR:O | 2.20 | 0.42 |
| 5:EI:89:TYR:HB3 | 5:EJ:98:VAL:HG13 | 2.01 | 0.42 |
| 5:EI:90:ASN:HD21 | 5:EJ:49:TRP:C | 2.19 | 0.42 |
| 5:EJ:215:PRO:HB3 | 5:EJ:229:ASN:C | 2.39 | 0.42 |
| 5:EJ:49:TRP:HH2 | 5:EJ:96:ARG:HE | 1.67 | 0.42 |
| 4:F:190:PRO:HA | 4:F:262:THR:HA | 2.01 | 0.42 |
| 5:FA:352:SER:HB2 | 5:FA:354:THR:O | 2.18 | 0.42 |
| 6:FB:86:ASP:CG | 6:FB:180:GLN:HE21 | 2.19 | 0.42 |
| 6:FC:71:ILE:O | 6:FC:215:PHE:N | 2.36 | 0.42 |
| 5:CF:348:THR:H | 7:FE:233:GLN:CG | 2.33 | 0.42 |
| 7:FF:66:VAL:HG21 | 7:FF:80:THR:HB | 2.01 | 0.42 |
| 7:FF:71:ASN:HB2 | 7:HJ:365:GLY:CA | 2.45 | 0.42 |
| 7:FG:232:THR:HG23 | 7:FG:234:SER:N | 2.34 | 0.42 |
| 8:FH:134:PRO:HA | 8:FH:157:LEU:HD23 | 2.01 | 0.42 |
| 9:FJ:47:ARG:HD2 | 9:FJ:47:ARG:HA | 1.79 | 0.42 |
| 4:G:251:ASN:N | 4:G:266:SER:O | 2.52 | 0.42 |
| 1:EB:66:TYR:OH | 11:GB:57:GLU:OE1 | 2.37 | 0.42 |
| 1:GE:199:LEU:HD21 | 1:GE:224:TYR:CG | 2.53 | 0.42 |
| 1:GE:341:THR:OG1 | 1:GE:342:ALA:N | 2.51 | 0.42 |
| 2:GF:18:ALA:HB2 | 2:GF:103:PHE:O | 2.19 | 0.42 |
| 2:GF:146:LEU:HA | 2:GF:585:MET:HA | 2.02 | 0.42 |
| 2:GF:416:VAL:HG23 | 2:GF:417:PHE:H | 1.84 | 0.42 |
| 2:GF:584:GLY:HA2 | 2:GF:600:PHE:CB | 2.46 | 0.42 |
| 2:GF:653:MET:SD | 2:GF:654:PRO:HD2 | 2.59 | 0.42 |
| 2:GF:798:ILE:HG12 | 2:GF:811:VAL:HG12 | 2.00 | 0.42 |
| 3:GG:140:GLY:HA2 | 3:GG:163:SER:OG | 2.19 | 0.42 |
| 3:GH:294:LYS:HB2 | 3:GH:297:TYR:CZ | 2.53 | 0.42 |
| 5:HB:134:GLU:O | 5:HB:145:TYR:HA | 2.19 | 0.42 |
| 5:HB:89:TYR:CD1 | 5:HB:139:ALA:HA | 2.54 | 0.42 |
| 5:HB:166:GLU:N | 5:HB:166:GLU:OE1 | 2.52 | 0.42 |
| 5:HB:323:THR:CG2 | 5:HB:354:THR:HG23 | 2.48 | 0.42 |
| 5:HB:558:ASP:O | 5:HB:566:TYR:HE2 | 2.02 | 0.42 |
| 5:HD:102:TRP:CZ3 | 5:HD:131:SER:HB2 | 2.53 | 0.42 |
| 5:HD:71:ASN:ND2 | 5:HD:73:SER:OG | 2.52 | 0.42 |
| 6:HE:82:VAL:HG23 | 6:HE:187:LYS:HE3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:HF:64:ILE:HG23 | 6:HF:217:ARG:HH12 | 1.84 | 0.42 |
| 7:HH:161:THR:OG1 | 7:HI:155:ASP:O | 2.25 | 0.42 |
| 5:I:137:TYR:HA | 5:I:143:TRP:HD1 | 1.84 | 0.42 |
| 5:I:149:LYS:HB2 | 5:J:153:LYS:HZ3 | 1.85 | 0.42 |
| 5:I:150:GLN:HG3 | 5:I:151:ILE:O | 2.18 | 0.42 |
| 5:I:558:ASP:O | 5:I:566:TYR:HE2 | 2.02 | 0.42 |
| 8:IB:88:TRP:CE3 | 8:IB:134:PRO:HD3 | 2.53 | 0.42 |
| 8:IB:25:ILE:O | 8:IB:26:SER:HB3 | 2.19 | 0.42 |
| 8:S:133:TRP:CH2 | 8:IB:61:ALA:HB2 | 2.54 | 0.42 |
| 9:IC:108:ILE:O | 9:IC:121:GLN:HA | 2.19 | 0.42 |
| 5:J:150:GLN:C | 5:J:151:ILE:HG13 | 2.40 | 0.42 |
| 5:K:207:SER:O | 5:K:210:SER:OG | 2.32 | 0.42 |
| 5:K:215:PRO:HB3 | 5:K:229:ASN:O | 2.19 | 0.42 |
| 5:K:320:LEU:HG | 5:K:357:SER:CB | 2.49 | 0.42 |
| 6:L:6:ASN:HB3 | 6:M:12:SER:CB | 2.49 | 0.42 |
| 6:N:217:ARG:HE | 6:N:219:ALA:C | 2.23 | 0.42 |
| 7:O:435:GLY:HA2 | 7:Q:517:ILE:HD11 | 2.01 | 0.42 |
| 7:O:251:ASN:HB2 | 7:P:253:ARG:HH22 | 1.84 | 0.42 |
| 7:P:347:MET:HE3 | 7:P:347:MET:HB2 | 1.77 | 0.42 |
| 7:P:451:PHE:HD1 | 7:P:469:VAL:HG13 | 1.85 | 0.42 |
| 7:P:477:TRP:CZ3 | 7:Q:469:VAL:HB | 2.54 | 0.42 |
| 7:P:77:THR:OG1 | 7:P:78:PRO:HD2 | 2.19 | 0.42 |
| 7:O:257:THR:HA | 7:Q:265:LEU:O | 2.19 | 0.42 |
| 1:Y:209:TRP:O | 1:Y:210:THR:C | 2.58 | 0.42 |
| 1:Y:403:PRO:HB2 | 2:Z:888:PHE:CD2 | 2.54 | 0.42 |
| 1:Y:610:ASN:ND2 | 2:Z:804:ASN:HA | 2.33 | 0.42 |
| 13:YA:195[A]:GLU:HG2 | 13:YA:197[A]:TYR:CE2 | 2.54 | 0.42 |
| 13:YA:277[C]:LEU:HD23 | 13:YA:277[C]:LEU:HA | 1.80 | 0.42 |
| 13:YA:320[C]:THR:HG22 | 13:YA:323[C]:ARG:HB3 | 2.00 | 0.42 |
| 13:YA:389[A]:TYR:O | 13:YA:405[A]:ASP:HB2 | 2.19 | 0.42 |
| 13:YA:454[A]:LYS:C | 13:YA:455[A]:LYS:HG3 | 2.39 | 0.42 |
| 13:YA:454[E]:LYS:C | 13:YA:455[E]:LYS:HG3 | 2.39 | 0.42 |
| 13:YA:38[B]:GLN:O | 13:YA:46[B]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:534[B]:LEU:HD11 | 13:YA:536[B]:TRP:NE1 | 2.32 | 0.42 |
| 13:YA:564[F]:GLN:HG3 | 13:YA:566[F]:THR:HG22 | 2.01 | 0.42 |
| 13:YA:83[F]:TYR:OH | 13:YA:85[F]:HIS:HE1 | 2.02 | 0.42 |
| 13:YB:147[D]:ILE:HD11 | 13:YB:188[D]:LEU:HG | 2.00 | 0.42 |
| 13:YB:200[A]:ILE:HD13 | 13:YB:236[A]:ILE:HD12 | 2.01 | 0.42 |
| 13:YB:389[F]:TYR:O | 13:YB:405[F]:ASP:HB2 | 2.18 | 0.42 |
| 13:YB:439[F]:TYR:HB3 | 13:YB:441[F]:ILE:CD1 | 2.49 | 0.42 |
| 13:YB:454[C]:LYS:C | 13:YB:455[C]:LYS:HG3 | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:454[E]:LYS:NZ | 13:YC:464[E]:TYR:OH | 2.53 | 0.42 |
| 13:YB:540[D]:GLY:HA3 | 13:YC:533[D]:ASN:ND2 | 2.22 | 0.42 |
| 13:YB:552[D]:GLU:CG | 13:YB:554[D]:MET:HE1 | 2.49 | 0.42 |
| 13:YC:195[E]:GLU:HG2 | 13:YC:197[E]:TYR:CE2 | 2.54 | 0.42 |
| 13:YC:336[A]:LEU:HA | 13:YC:336[A]:LEU:HD12 | 1.84 | 0.42 |
| 13:YC:38[C]:GLN:O | 13:YC:46[C]:GLY:HA2 | 2.20 | 0.42 |
| 13:YC:389[B]:TYR:O | 13:YC:405[B]:ASP:HB2 | 2.19 | 0.42 |
| 13:YB:546[C]:VAL:HG11 | 13:YC:542[C]:VAL:HG13 | 2.01 | 0.42 |
| 14:YD:114[F]:SER:HA | 14:YD:167[F]:GLU:OE1 | 2.19 | 0.42 |
| 14:YD:73[D]:SER:HA | 14:YD:85[D]:THR:HA | 2.01 | 0.42 |
| 14:YE:112[E]:ILE:HB | 14:YE:140[E]:TYR:OH | 2.19 | 0.42 |
| 14:YE:170[F]:LEU:HD23 | 14:YE:170[F]:LEU:HA | 1.69 | 0.42 |
| 14:YE:172[B]:TYR:CZ | 14:YE:176[B]:VAL:HG21 | 2.54 | 0.42 |
| 14:YE:75[A]:ALA:HB2 | 14:YE:83[A]:VAL:HA | 2.00 | 0.42 |
| 14:YF:112[D]:ILE:HB | 14:YF:140[D]:TYR:OH | 2.19 | 0.42 |
| 14:YF:112[F]:ILE:HB | 14:YF:140[F]:TYR:OH | 2.19 | 0.42 |
| 14:YF:17[B]:PHE:HE2 | 14:YF:26[B]:ASN:HA | 1.85 | 0.42 |
| 14:YF:43[D]:SER:O | 14:YF:189[D]:TRP:HB2 | 2.20 | 0.42 |
| 14:YF:238[C]:THR:N | 14:YF:307[C]:TYR:O | 2.52 | 0.42 |
| 11:GB:182:ASN:ND2 | 14:YF:327[A]:ASN:HD22 | 2.17 | 0.42 |
| 2:Z:494:GLU:HB2 | 2:Z:498:TRP:CB | 2.49 | 0.42 |
| 2:Z:572:ASN:CB | 2:Z:611:ILE:HG22 | 2.48 | 0.42 |
| 2:Z:669:GLU:O | 2:Z:672:ILE:N | 2.51 | 0.42 |
| 2:Z:981:GLN:CG | 2:Z:982:LEU:N | 2.81 | 0.42 |
| 15:ZA:37[E]:LEU:HB2 | 15:ZA:75[E]:VAL:HB | 2.01 | 0.42 |
| 1:A:414:LEU:HD23 | 1:A:486:ARG:HE | 1.85 | 0.42 |
| 1:A:494:THR:HG22 | 1:A:498:GLY:HA2 | 2.01 | 0.42 |
| 4:AB:224:ASP:OD2 | 4:AB:227:ASN:HB2 | 2.19 | 0.42 |
| 4:AB:43:GLY:HA2 | 4:AB:62:HIS:CE1 | 2.55 | 0.42 |
| 5:AC:107:VAL:HB | 5:AC:126:ILE:HB | 2.01 | 0.42 |
| 5:AC:89:TYR:CD1 | 5:AC:139:ALA:HA | 2.54 | 0.42 |
| 5:AC:336:SER:HB3 | 5:AC:348:THR:O | 2.20 | 0.42 |
| 5:AD:116:THR:HG22 | 5:AD:121:ALA:HB2 | 2.02 | 0.42 |
| 5:AE:180:VAL:HG22 | 5:AE:181:PHE:H | 1.84 | 0.42 |
| 5:AE:186:TYR:HB3 | 5:AE:227:GLY:CA | 2.49 | 0.42 |
| 5:AE:215:PRO:HB3 | 5:AE:229:ASN:C | 2.40 | 0.42 |
| 5:AE:288:MET:CE | 5:AE:292:PRO:HD3 | 2.50 | 0.42 |
| 5:AC:555:CYS:O | 5:AE:557:TYR:HE1 | 2.02 | 0.42 |
| 5:AE:79:ILE:HD12 | 5:AE:81:LEU:HD11 | 2.01 | 0.42 |
| 5:AE:89:TYR:C | 5:AE:91:LYS:H | 2.23 | 0.42 |
| 6:AG:135:GLU:O | 6:AG:139:SER:N | 2.26 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AG:64:ILE:HG23 | 6:AG:217:ARG:HH12 | 1.84 | 0.42 |
| 7:AI:139:ASN:N | 7:BA:143:LYS:HG2 | 2.34 | 0.42 |
| 7:AI:378:ARG:NH1 | 7:BA:355:PRO:HG3 | 2.34 | 0.42 |
| 7:AJ:480:ARG:CZ | 7:BA:465:ARG:HG3 | 2.49 | 0.42 |
| 7:AJ:359:TRP:CH2 | 7:AJ:524:LYS:HB2 | 2.54 | 0.42 |
| 5:AD:200:LEU:HB2 | 7:AJ:5:THR:HG21 | 2.01 | 0.42 |
| 1:B:346:ASP:O | 1:B:350:SER:N | 2.50 | 0.42 |
| 1:B:378:PRO:O | 1:B:379:LYS:HG2 | 2.19 | 0.42 |
| 1:B:530:LEU:HD12 | 1:B:532:GLU:H | 1.84 | 0.42 |
| 7:BA:20:PRO:CG | 7:BA:29:ILE:HG13 | 2.49 | 0.42 |
| 8:BC:25:ILE:O | 8:BC:26:SER:HB3 | 2.19 | 0.42 |
| 10:BE:133:LYS:HB3 | 10:BE:208:THR:O | 2.20 | 0.42 |
| 12:BG:140:ASP:OD1 | 12:BG:141:TRP:N | 2.52 | 0.42 |
| 1:BH:365:ASP:OD2 | 1:BH:367:THR:HB | 2.18 | 0.42 |
| 1:BH:609:ILE:HG22 | 1:BH:611:LEU:HG | 2.01 | 0.42 |
| 1:BH:64:THR:HG21 | 2:BJ:674:TYR:HE2 | 1.85 | 0.42 |
| 1:BI:448:TYR:HA | 1:BI:452:VAL:CG1 | 2.49 | 0.42 |
| 2:BJ:416:VAL:HG23 | 2:BJ:417:PHE:H | 1.84 | 0.42 |
| 2:BJ:478:GLU:HG3 | 2:BJ:488:MET:SD | 2.58 | 0.42 |
| 2:BJ:548:ILE:HG21 | 2:BJ:555:ARG:H | 1.84 | 0.42 |
| 2:C:1005:ARG:HG2 | 2:C:1006:ASP:O | 2.19 | 0.42 |
| 2:C:114:ILE:HG23 | 2:C:115:GLU:H | 1.83 | 0.42 |
| 2:C:457:ASN:O | 2:C:458:ASP:C | 2.58 | 0.42 |
| 2:C:694:TYR:HD2 | 2:C:696:ARG:N | 2.05 | 0.42 |
| 3:CA:115:ASN:HD21 | 3:CA:123:GLU:HB3 | 1.83 | 0.42 |
| 3:CA:131:TYR:HD1 | 3:CA:190:TYR:HA | 1.84 | 0.42 |
| 3:CB:254:ASP:CG | 3:CB:256:VAL:HG12 | 2.39 | 0.42 |
| 4:CC:168:PHE:CE1 | 4:CD:161:ASN:HB3 | 2.54 | 0.42 |
| 4:CD:251:ASN:N | 4:CD:266:SER:O | 2.53 | 0.42 |
| 4:CD:209:VAL:HG13 | 4:CD:271:GLY:O | 2.19 | 0.42 |
| 4:CE:100:ARG:NH2 | 4:CE:128:ASP:OD1 | 2.53 | 0.42 |
| 4:CE:44:ASP:O | 4:CE:59:GLN:NE2 | 2.52 | 0.42 |
| 5:CF:137:TYR:HA | 5:CF:143:TRP:HD1 | 1.84 | 0.42 |
| 5:CG:153:LYS:HG2 | 5:CG:154:ILE:N | 2.32 | 0.42 |
| 5:CG:257:SER:O | 5:CG:258:TYR:HB3 | 2.20 | 0.42 |
| 5:CH:151:ILE:HG23 | 5:CH:152:ASP:N | 2.34 | 0.42 |
| 5:CH:368:ILE:HG13 | 5:CH:369:LEU:N | 2.35 | 0.42 |
| 6:CJ:82:VAL:HG23 | 6:CJ:187:LYS:HE3 | 2.01 | 0.42 |
| 6:DA:87:TYR:N | 6:DA:181:GLU:O | 2.32 | 0.42 |
| 7:DB:466:SER:HB3 | 7:DB:468:PHE:CE2 | 2.54 | 0.42 |
| 7:DC:117:THR:HB | 7:DD:112:ASN:HA | 1.99 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DC:118:PRO:HB3 | 7:DD:106:ALA:O | 2.18 | 0.42 |
| 7:DC:228:ILE:O | 7:DD:226:GLY:N | 2.49 | 0.42 |
| 7:DC:480:ARG:CZ | 7:DD:465:ARG:HG3 | 2.49 | 0.42 |
| 7:DC:480:ARG:HD3 | 7:DD:462:ASN:ND2 | 2.35 | 0.42 |
| 7:DB:435:GLY:HA2 | 7:DD:517:ILE:HD11 | 2.01 | 0.42 |
| 11:DI:55:ARG:HD2 | 11:DI:55:ARG:HA | 1.83 | 0.42 |
| 1:EA:278:ALA:H | 1:EA:316:GLY:HA2 | 1.85 | 0.42 |
| 1:EB:371:TYR:HB3 | 1:EB:373:PHE:CE1 | 2.54 | 0.42 |
| 1:EB:373:PHE:O | 1:EB:374:ILE:HD13 | 2.18 | 0.42 |
| 1:EB:619:GLN:CD | 1:EB:619:GLN:H | 2.21 | 0.42 |
| 2:EC:108:TYR:CD2 | 2:EC:108:TYR:N | 2.87 | 0.42 |
| 2:EC:457:ASN:O | 2:EC:458:ASP:C | 2.58 | 0.42 |
| 2:EC:701:TRP:O | 2:EC:701:TRP:CG | 2.72 | 0.42 |
| 2:EC:761:GLU:HB2 | 2:EC:862:TYR:CE1 | 2.54 | 0.42 |
| 3:ED:115:ASN:HD21 | 3:ED:123:GLU:HB3 | 1.83 | 0.42 |
| 3:EE:228:ASN:HA | 3:EE:229:LEU:HD13 | 2.01 | 0.42 |
| 5:EI:185:SER:HB2 | 5:EI:228:PHE:HE1 | 1.84 | 0.42 |
| 5:EI:222:LEU:HD11 | 5:EI:224:PRO:HD2 | 2.01 | 0.42 |
| 5:EI:239:GLY:O | 7:FE:5:THR:N | 2.48 | 0.42 |
| 5:EI:322:GLY:HA2 | 5:EI:360:THR:N | 2.34 | 0.42 |
| 5:EI:558:ASP:O | 5:EI:566:TYR:HE2 | 2.02 | 0.42 |
| 5:FA:192:ARG:HB2 | 5:FA:245:GLU:H | 1.84 | 0.42 |
| 5:FA:322:GLY:CA | 5:FA:359:GLU:HA | 2.50 | 0.42 |
| 7:FE:378:ARG:NH1 | 7:FG:355:PRO:HG3 | 2.34 | 0.42 |
| 7:FE:363:HIS:CD2 | 7:FE:396:ARG:HD3 | 2.54 | 0.42 |
| 7:FE:402:GLY:O | 7:FG:397:GLY:N | 2.46 | 0.42 |
| 7:FG:29:ILE:HG23 | 7:FG:29:ILE:HD12 | 1.76 | 0.42 |
| 7:FG:349:TRP:NE1 | 7:FG:351:ALA:HB3 | 2.34 | 0.42 |
| 7:FG:47:VAL:HG12 | 7:FG:48:PRO:N | 2.35 | 0.42 |
| 7:FE:463:THR:HG23 | 7:FG:483:PHE:HE1 | 1.84 | 0.42 |
| 8:FH:69:TRP:CZ3 | 8:FH:157:LEU:HD12 | 2.51 | 0.42 |
| 10:GA:286:VAL:HG13 | 14:YE:100[E]:LYS:HE2 | 2.01 | 0.42 |
| 1:GD:157:LYS:O | 1:GD:158:ASN:CG | 2.57 | 0.42 |
| 1:GD:508:ARG:HH22 | 1:GD:577:PHE:HA | 1.84 | 0.42 |
| 1:GD:494:THR:OG1 | 1:GD:604:TRP:O | 2.23 | 0.42 |
| 1:GE:116:ASP:HB2 | 1:GE:161:TYR:HE2 | 1.84 | 0.42 |
| 2:GF:314:THR:HG23 | 2:GF:317:TYR:HB2 | 2.01 | 0.42 |
| 2:GF:613:LYS:HG3 | 2:GF:614:PRO:HD3 | 2.00 | 0.42 |
| 2:GF:927:THR:HB | 2:GF:987:ARG:HA | 2.00 | 0.42 |
| 3:GG:16:PHE:HB2 | 3:GH:310:ILE:HB | 2.01 | 0.42 |
| 4:GI:124:ILE:HB | 4:GI:137:LEU:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:GI:224:ASP:OD2 | 4:GI:227:ASN:HB2 | 2.19 | 0.42 |
| 4:GI:7:LYS:O | 4:HA:54:THR:HA | 2.19 | 0.42 |
| 4:GJ:43:GLY:HA2 | 4:GJ:62:HIS:CE1 | 2.55 | 0.42 |
| 4:HA:67:TYR:CD1 | 4:HA:84:ARG:HB3 | 2.50 | 0.42 |
| 5:HB:302:GLU:HG3 | 5:HB:303:PRO:HD2 | 2.00 | 0.42 |
| 5:HB:424:ASP:OD2 | 5:HB:427:LYS:HB3 | 2.19 | 0.42 |
| 5:HC:129:ARG:HG3 | 5:HC:130:PHE:N | 2.33 | 0.42 |
| 5:HC:102:TRP:HE3 | 5:HC:131:SER:HB2 | 1.84 | 0.42 |
| 5:HC:150:GLN:C | 5:HC:151:ILE:HG13 | 2.40 | 0.42 |
| 5:HC:304:ILE:HD11 | 5:HC:309:LEU:HA | 2.00 | 0.42 |
| 5:HC:328:LEU:HG | 5:HC:329:PHE:H | 1.84 | 0.42 |
| 5:HD:215:PRO:HB3 | 5:HD:229:ASN:C | 2.40 | 0.42 |
| 5:HC:399:ILE:HD13 | 5:HD:399:ILE:HG22 | 2.01 | 0.42 |
| 6:HF:217:ARG:HE | 6:HF:219:ALA:C | 2.23 | 0.42 |
| 6:HG:201:VAL:N | 6:HG:210:THR:O | 2.31 | 0.42 |
| 7:HH:176:ILE:HG23 | 7:HH:177:ALA:H | 1.84 | 0.42 |
| 7:HH:260:ARG:HD3 | 7:HJ:262:VAL:HG23 | 2.00 | 0.42 |
| 7:HI:103:ASN:OD1 | 7:HI:120:LYS:HG2 | 2.19 | 0.42 |
| 7:HI:146:SER:HB2 | 7:HI:149:GLN:HG2 | 2.01 | 0.42 |
| 7:HH:97:LEU:HD22 | 7:HI:96:GLY:HA2 | 1.99 | 0.42 |
| 7:HH:185:GLU:HA | 7:HJ:193:LEU:HB2 | 2.01 | 0.42 |
| 7:HJ:20:PRO:CG | 7:HJ:29:ILE:HG13 | 2.49 | 0.42 |
| 5:I:89:TYR:CD1 | 5:I:139:ALA:HA | 2.54 | 0.42 |
| 5:I:416:ILE:HG23 | 5:K:472:TYR:HA | 2.00 | 0.42 |
| 5:I:424:ASP:OD2 | 5:I:427:LYS:HB3 | 2.19 | 0.42 |
| 12:IF:140:ASP:OD1 | 12:IF:141:TRP:N | 2.52 | 0.42 |
| 5:J:267:ASP:H | 5:J:377:HIS:HB2 | 1.84 | 0.42 |
| 5:K:368:ILE:HG13 | 5:K:369:LEU:N | 2.35 | 0.42 |
| 5:I:555:CYS:O | 5:K:557:TYR:HE1 | 2.02 | 0.42 |
| 5:K:58:GLN:N | 5:K:58:GLN:OE1 | 2.37 | 0.42 |
| 7:O:464:ARG:NH2 | 7:P:492:PRO:HD2 | 2.33 | 0.42 |
| 7:P:116:ILE:HG23 | 7:P:120:LYS:HB2 | 2.00 | 0.42 |
| 7:Q:101:SER:OG | 7:Q:102:THR:N | 2.52 | 0.42 |
| 7:P:173:ILE:CG2 | 7:Q:173:ILE:HG12 | 2.43 | 0.42 |
| 7:Q:196:VAL:HG22 | 7:Q:214:THR:HG22 | 2.02 | 0.42 |
| 7:Q:472:ARG:NE | 5:FA:363:ASN:HD21 | 2.16 | 0.42 |
| 7:Q:47:VAL:HG12 | 7:Q:48:PRO:N | 2.34 | 0.42 |
| 1:X:494:THR:HG22 | 1:X:498:GLY:HA2 | 2.01 | 0.42 |
| 1:Y:654:ASP:OD1 | 1:Y:655:LEU:N | 2.52 | 0.42 |
| 13:YA:195[B]:GLU:HG2 | 13:YA:197[B]:TYR:CE2 | 2.54 | 0.42 |
| 13:YA:195[C]:GLU:HG2 | 13:YA:197[C]:TYR:CE2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:236[F]:ILE:HG23 | 13:YA:240[F]:GLU:HB2 | 1.99 | 0.42 |
| 13:YA:257[A]:LYS:HE2 | 13:YA:266[A]:TRP:CH2 | 2.53 | 0.42 |
| 13:YA:330[D]:ILE:HD12 | 13:YA:336[D]:LEU:HD12 | 2.01 | 0.42 |
| 13:YB:154[C]:THR:H | 13:YB:182[C]:ARG:NH2 | 2.17 | 0.42 |
| 13:YB:195[F]:GLU:HG2 | 13:YB:197[F]:TYR:CE2 | 2.55 | 0.42 |
| 13:YB:236[D]:ILE:HG23 | 13:YB:240[D]:GLU:HB2 | 1.99 | 0.42 |
| 13:YB:257[E]:LYS:HE2 | 13:YB:266[E]:TRP:CH2 | 2.53 | 0.42 |
| 13:YB:26[C]:ARG:HD3 | 14:YE:259[C]:LEU:HD21 | 2.00 | 0.42 |
| 13:YB:327[F]:VAL:O | 13:YB:331[F]:ILE:HG22 | 2.20 | 0.42 |
| 13:YB:327[C]:VAL:O | 13:YB:331[C]:ILE:HG22 | 2.20 | 0.42 |
| 13:YB:389[A]:TYR:O | 13:YB:405[A]:ASP:HB2 | 2.19 | 0.42 |
| 13:YB:439[E]:TYR:HB3 | 13:YB:441[E]:ILE:CD1 | 2.50 | 0.42 |
| 13:YA:376[D]:PHE:CD2 | 13:YB:447[D]:ASN:OD1 | 2.71 | 0.42 |
| 13:YA:560[A]:ILE:O | 13:YB:553[A]:LYS:HA | 2.18 | 0.42 |
| 13:YB:83[B]:TYR:OH | 13:YB:85[B]:HIS:HE1 | 2.02 | 0.42 |
| 13:YC:127[A]:ASN:ND2 | 13:YC:129[A]:THR:OG1 | 2.53 | 0.42 |
| 13:YC:195[A]:GLU:HG2 | 13:YC:197[A]:TYR:CE2 | 2.54 | 0.42 |
| 13:YC:280[E]:MET:O | 13:YC:284[E]:MET:HG2 | 2.19 | 0.42 |
| 13:YC:330[A]:ILE:HD12 | 13:YC:336[A]:LEU:HD12 | 2.01 | 0.42 |
| 13:YC:439[D]:TYR:HB3 | 13:YC:441[D]:ILE:CD1 | 2.49 | 0.42 |
| 13:YB:454[C]:LYS:NZ | 13:YC:464[C]:TYR:OH | 2.52 | 0.42 |
| 13:YC:38[D]:GLN:O | 13:YC:46[D]:GLY:HA2 | 2.20 | 0.42 |
| 13:YC:534[D]:LEU:HD11 | 13:YC:536[D]:TRP:NE1 | 2.32 | 0.42 |
| 13:YA:530[B]:VAL:O | 13:YC:538[B]:VAL:HA | 2.19 | 0.42 |
| 13:YC:58[C]:ILE:HG12 | 13:YC:97[C]:LEU:HD22 | 2.01 | 0.42 |
| 14:YD:114[B]:SER:HA | 14:YD:167[B]:GLU:OE1 | 2.20 | 0.42 |
| 14:YD:112[E]:ILE:HB | 14:YD:140[E]:TYR:OH | 2.19 | 0.42 |
| 14:YD:15[B]:LYS:HE2 | 14:YD:15[B]:LYS:HB3 | 1.54 | 0.42 |
| 14:YD:308[C]:ALA:O | 14:YD:357[C]:MET:N | 2.52 | 0.42 |
| 14:YD:75[A]:ALA:HB2 | 14:YD:83[A]:VAL:HA | 2.00 | 0.42 |
| 14:YE:112[B]:ILE:HB | 14:YE:140[B]:TYR:OH | 2.20 | 0.42 |
| 14:YE:15[F]:LYS:HB3 | 14:YE:15[F]:LYS:HE2 | 1.54 | 0.42 |
| 14:YE:234[C]:PHE:HD1 | 14:YF:97[C]:VAL:HG12 | 1.83 | 0.42 |
| 14:YE:301[C]:MET:O | 14:YE:304[C]:TYR:N | 2.49 | 0.42 |
| 14:YE:373[C]:LYS:HB3 | 14:YE:373[C]:LYS:HE2 | 1.87 | 0.42 |
| 14:YF:112[E]:ILE:HB | 14:YF:140[E]:TYR:OH | 2.19 | 0.42 |
| 14:YF:114[D]:SER:HA | 14:YF:167[D]:GLU:OE1 | 2.20 | 0.42 |
| 13:YC:47[D]:ILE:HG12 | 14:YF:123[D]:PRO:HD3 | 2.00 | 0.42 |
| 14:YF:172[C]:TYR:CZ | 14:YF:176[C]:VAL:HG21 | 2.55 | 0.42 |
| 14:YF:132[A]:ILE:HD12 | 14:YF:197[A]:MET:SD | 2.59 | 0.42 |
| 14:YF:17[D]:PHE:HE2 | 14:YF:26[D]:ASN:HA | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:277[A]:VAL:HG11 | 14:YF:294[A]:GLU:HG2 | 1.99 | 0.42 |
| 14:YF:364[F]:LEU:HA | 14:YF:364[F]:LEU:HD22 | 1.80 | 0.42 |
| 14:YE:242[C]:PRO:HD2 | 14:YF:91[C]:LYS:O | 2.19 | 0.42 |
| 2:Z:108:TYR:N | 2:Z:108:TYR:CD2 | 2.87 | 0.42 |
| 2:Z:980:GLY:C | 2:Z:983:PRO:HD2 | 2.40 | 0.42 |
| 1:A:491:PHE:CE2 | 1:A:619:GLN:HA | 2.55 | 0.42 |
| 4:AB:100:ARG:NH2 | 4:AB:128:ASP:OD1 | 2.53 | 0.42 |
| 5:AC:170:GLU:O | 5:AC:171:VAL:HG12 | 2.19 | 0.42 |
| 5:AC:229:ASN:OD1 | 5:AC:230:ILE:N | 2.51 | 0.42 |
| 5:AD:153:LYS:HG2 | 5:AD:154:ILE:N | 2.32 | 0.42 |
| 5:AD:180:VAL:HG22 | 5:AD:181:PHE:H | 1.84 | 0.42 |
| 5:AD:215:PRO:HB3 | 5:AD:229:ASN:C | 2.39 | 0.42 |
| 5:AD:275:SER:OG | 5:AD:281:TYR:HA | 2.18 | 0.42 |
| 5:AD:389:ASP:OD1 | 5:AD:389:ASP:N | 2.51 | 0.42 |
| 5:AD:430:TRP:HA | 5:AD:431:PRO:C | 2.40 | 0.42 |
| 5:AD:478:TRP:CH2 | 5:AD:600:ARG:HB2 | 2.54 | 0.42 |
| 5:AE:304:ILE:HD12 | 5:AE:306:PRO:HA | 2.02 | 0.42 |
| 6:AG:44:ALA:HA | 6:AH:110:PHE:C | 2.40 | 0.42 |
| 6:AG:88:TRP:O | 6:AG:155:LYS:HA | 2.18 | 0.42 |
| 7:AI:464:ARG:NH2 | 7:AJ:492:PRO:HD2 | 2.34 | 0.42 |
| 7:AI:497:ASN:OD1 | 7:AI:500:TYR:N | 2.53 | 0.42 |
| 1:B:521:ARG:HB2 | 1:B:533:ASP:CG | 2.39 | 0.42 |
| 1:B:539:ARG:O | 1:B:541:VAL:HG23 | 2.19 | 0.42 |
| 7:BA:21:THR:OG1 | 7:BA:22:ASP:N | 2.51 | 0.42 |
| 7:BA:85:LEU:O | 7:BA:86:SER:OG | 2.21 | 0.42 |
| 9:BD:85:GLU:OE2 | 9:BD:87:ARG:NH2 | 2.53 | 0.42 |
| 11:BF:107:ASP:HA | 11:BF:155:THR:HG22 | 2.00 | 0.42 |
| 1:BI:148:ARG:HG2 | 1:BI:149:GLU:HG3 | 2.01 | 0.42 |
| 1:BI:377:LYS:HB3 | 1:BI:377:LYS:HE2 | 1.65 | 0.42 |
| 1:BI:423:THR:O | 1:BI:476:ILE:N | 2.45 | 0.42 |
| 1:BI:448:TYR:HD1 | 1:BI:452:VAL:HG11 | 1.85 | 0.42 |
| 1:BI:596:ASN:OD1 | 1:BI:596:ASN:N | 2.53 | 0.42 |
| 1:BI:60:LEU:HD23 | 1:BI:60:LEU:HA | 1.73 | 0.42 |
| 2:BJ:139:ASN:HA | 2:BJ:555:ARG:NH2 | 2.34 | 0.42 |
| 2:BJ:494:GLU:HB2 | 2:BJ:498:TRP:CB | 2.49 | 0.42 |
| 2:BJ:761:GLU:HB2 | 2:BJ:862:TYR:CE1 | 2.54 | 0.42 |
| 2:C:186:ASP:HB3 | 2:C:189:ARG:HE | 1.83 | 0.42 |
| 2:C:603:ARG:HH12 | 1:Y:390:GLU:HG2 | 1.84 | 0.42 |
| 3:CA:71:MET:HB2 | 3:CA:71:MET:HE2 | 1.90 | 0.42 |
| 3:CB:175:ASP:OD1 | 3:CB:176:ALA:N | 2.48 | 0.42 |
| 4:CC:28:GLY:O | 4:CC:32:ASN:ND2 | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:275:SER:OG | 5:CF:282:VAL:N | 2.52 | 0.42 |
| 5:CH:304:ILE:HD12 | 5:CH:304:ILE:O | 2.20 | 0.42 |
| 3:D:254:ASP:HB3 | 3:D:257:TYR:HD2 | 1.84 | 0.42 |
| 5:CG:340:VAL:HG22 | 6:DA:173:THR:HA | 2.01 | 0.42 |
| 6:DA:217:ARG:HE | 6:DA:219:ALA:C | 2.23 | 0.42 |
| 7:DB:111:ASN:CG | 7:DB:114:SER:HB3 | 2.38 | 0.42 |
| 7:DB:257:THR:HA | 7:DD:265:LEU:O | 2.19 | 0.42 |
| 7:DB:346:ILE:N | 7:DD:348:MET:O | 2.28 | 0.42 |
| 7:DD:489:GLU:CD | 7:DD:502:LEU:H | 2.22 | 0.42 |
| 7:DD:493:GLU:HG3 | 7:DD:496:ARG:HH21 | 1.84 | 0.42 |
| 7:DD:58:LEU:HD21 | 7:DD:75:ALA:H | 1.84 | 0.42 |
| 8:DE:25:ILE:O | 8:DE:26:SER:HB3 | 2.20 | 0.42 |
| 12:DJ:15:ASP:CG | 12:DJ:16:PHE:N | 2.71 | 0.42 |
| 1:EA:90:VAL:HG11 | 1:EA:228:GLU:HG2 | 2.01 | 0.42 |
| 1:EB:403:PRO:HB2 | 2:EC:888:PHE:CD2 | 2.55 | 0.42 |
| 1:EB:429:LEU:HD12 | 1:EB:429:LEU:O | 2.19 | 0.42 |
| 1:EB:524:VAL:HG13 | 1:EB:529:GLY:O | 2.19 | 0.42 |
| 2:EC:222:VAL:HG12 | 2:EC:224:LEU:HB2 | 2.01 | 0.42 |
| 2:EC:653:MET:SD | 2:EC:654:PRO:HD2 | 2.59 | 0.42 |
| 2:EC:725:ARG:HA | 2:EC:728:GLU:HB3 | 2.00 | 0.42 |
| 3:ED:71:MET:HE2 | 3:ED:71:MET:HB2 | 1.88 | 0.42 |
| 3:EE:104:TYR:CB | 3:EE:165:ARG:HB2 | 2.50 | 0.42 |
| 4:EF:131:LYS:HD3 | 4:EF:161:ASN:HD22 | 1.85 | 0.42 |
| 4:EF:190:PRO:HA | 4:EF:262:THR:HA | 2.01 | 0.42 |
| 4:EG:100:ARG:NH2 | 4:EG:128:ASP:OD1 | 2.53 | 0.42 |
| 5:EI:22:GLY:O | 5:EI:26:ILE:N | 2.37 | 0.42 |
| 5:EI:469:PRO:HA | 5:EI:472:TYR:CZ | 2.54 | 0.42 |
| 5:EI:36:GLU:OE1 | 5:EI:66:LYS:HG2 | 2.19 | 0.42 |
| 5:EJ:267:ASP:H | 5:EJ:377:HIS:HB2 | 1.84 | 0.42 |
| 5:EJ:305:ASN:HB3 | 5:FA:255:ARG:NH1 | 2.34 | 0.42 |
| 5:EJ:54:ALA:HB2 | 5:EJ:71:ASN:O | 2.20 | 0.42 |
| 5:FA:89:TYR:CE1 | 5:FA:139:ALA:HA | 2.54 | 0.42 |
| 6:FD:90:PHE:CD2 | 6:FD:126:VAL:HG22 | 2.45 | 0.42 |
| 6:FD:82:VAL:HG23 | 6:FD:187:LYS:HE3 | 2.01 | 0.42 |
| 7:FE:143:LYS:HG2 | 7:FF:138:SER:C | 2.40 | 0.42 |
| 7:FE:397:GLY:HA2 | 7:FF:401:ARG:HE | 1.85 | 0.42 |
| 7:FF:99:ARG:HH11 | 7:FF:111:ASN:ND2 | 2.17 | 0.42 |
| 7:FG:20:PRO:CB | 7:FG:29:ILE:HG13 | 2.48 | 0.42 |
| 7:FG:425:LEU:HA | 7:FG:425:LEU:HD23 | 1.82 | 0.42 |
| 7:FG:85:LEU:CG | 7:FG:86:SER:H | 2.30 | 0.42 |
| 8:FI:134:PRO:HA | 8:FI:157:LEU:HD23 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:GC:118:TYR:CG | 12:GC:119:ASN:N | 2.86 | 0.42 |
| 1:GD:337:GLN:O | 1:GD:348:PHE:HZ | 2.02 | 0.42 |
| 1:GD:430:GLN:OE1 | 1:GD:430:GLN:N | 2.29 | 0.42 |
| 1:GE:178:ILE:HD12 | 1:GE:178:ILE:HA | 1.90 | 0.42 |
| 5:HB:358:VAL:HG23 | 5:HB:371:PHE:HD1 | 1.83 | 0.42 |
| 5:HB:64:TRP:CZ2 | 5:HB:82:PRO:HB2 | 2.54 | 0.42 |
| 5:HC:116:THR:HG22 | 5:HC:121:ALA:HB2 | 2.02 | 0.42 |
| 5:HC:153:LYS:HG2 | 5:HC:154:ILE:N | 2.32 | 0.42 |
| 5:HC:180:VAL:HG22 | 5:HC:181:PHE:H | 1.84 | 0.42 |
| 5:HC:199:GLU:OE1 | 5:HD:196:ARG:NH2 | 2.52 | 0.42 |
| 5:HC:483:GLN:O | 5:HC:485:LYS:HG2 | 2.20 | 0.42 |
| 5:HC:49:TRP:N | 5:HC:49:TRP:CD1 | 2.87 | 0.42 |
| 5:HC:98:VAL:HG12 | 5:HC:99:PHE:CD2 | 2.46 | 0.42 |
| 5:HD:151:ILE:HG23 | 5:HD:152:ASP:N | 2.34 | 0.42 |
| 5:HD:192:ARG:HB2 | 5:HD:245:GLU:H | 1.84 | 0.42 |
| 5:HD:288:MET:CE | 5:HD:292:PRO:HD3 | 2.50 | 0.42 |
| 5:HD:299:ILE:HA | 5:HD:300:PRO:HD3 | 1.89 | 0.42 |
| 5:HD:491:ASN:OD1 | 5:HD:493:ASP:N | 2.48 | 0.42 |
| 5:HD:58:GLN:N | 5:HD:58:GLN:OE1 | 2.37 | 0.42 |
| 6:HF:82:VAL:HG23 | 6:HF:187:LYS:HE3 | 2.02 | 0.42 |
| 7:HH:197:ALA:O | 7:HH:201:GLN:HG3 | 2.20 | 0.42 |
| 7:HH:497:ASN:OD1 | 7:HH:500:TYR:N | 2.53 | 0.42 |
| 7:HH:141:VAL:HG23 | 7:HI:140:GLY:O | 2.19 | 0.42 |
| 7:HH:312:GLY:N | 7:HI:316:THR:O | 2.39 | 0.42 |
| 7:HI:46:GLY:O | 7:HI:47:VAL:HG23 | 2.19 | 0.42 |
| 7:HI:66:VAL:HG21 | 7:HI:80:THR:HB | 2.01 | 0.42 |
| 7:HJ:118:PRO:O | 7:HJ:122:THR:N | 2.41 | 0.42 |
| 7:HJ:493:GLU:HG3 | 7:HJ:496:ARG:HH21 | 1.84 | 0.42 |
| 5:I:265:LEU:HD22 | 5:I:281:TYR:HD2 | 1.84 | 0.42 |
| 5:I:355:ASP:OD1 | 5:I:356:TYR:N | 2.49 | 0.42 |
| 12:GC:149:ARG:HB2 | 10:ID:341:THR:HG21 | 2.01 | 0.42 |
| 10:ID:62:LEU:O | 10:ID:128:LEU:HD12 | 2.20 | 0.42 |
| 5:I:472:TYR:O | 5:J:416:ILE:HD12 | 2.19 | 0.42 |
| 5:J:68:TYR:HB2 | 5:J:70:ILE:HD11 | 2.00 | 0.42 |
| 5:K:169:VAL:O | 5:K:238:ILE:HA | 2.19 | 0.42 |
| 5:K:186:TYR:HB3 | 5:K:227:GLY:C | 2.40 | 0.42 |
| 5:K:71:ASN:ND2 | 5:K:73:SER:OG | 2.52 | 0.42 |
| 5:K:67:SER:HA | 5:K:94:ARG:HB2 | 2.01 | 0.42 |
| 6:L:195:LEU:HD13 | 6:L:215:PHE:CE1 | 2.52 | 0.42 |
| 6:L:198:ALA:O | 6:M:203:LEU:HB3 | 2.20 | 0.42 |
| 6:M:217:ARG:HE | 6:M:219:ALA:C | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:97:LEU:HD23 | 7:Q:97:LEU:CD2 | 2.49 | 0.42 |
| 7:O:192:GLN:HG3 | 7:P:188:GLN:CD | 2.39 | 0.42 |
| 7:P:359:TRP:CH2 | 7:P:524:LYS:HB2 | 2.54 | 0.42 |
| 7:P:66:VAL:HG21 | 7:P:80:THR:HB | 2.01 | 0.42 |
| 12:W:184:PRO:HA | 12:IF:153:ARG:NH2 | 2.34 | 0.42 |
| 12:W:236:ILE:HD11 | 12:IF:16:PHE:CB | 2.48 | 0.42 |
| 1:X:430:GLN:H | 1:X:430:GLN:CD | 2.14 | 0.42 |
| 1:Y:539:ARG:O | 1:Y:541:VAL:HG23 | 2.19 | 0.42 |
| 13:YA:187[A]:ARG:HA | 13:YA:187[A]:ARG:HD3 | 1.86 | 0.42 |
| 13:YA:296[C]:LEU:HD12 | 13:YA:296[C]:LEU:HA | 1.84 | 0.42 |
| 13:YA:320[B]:THR:HG22 | 13:YA:323[B]:ARG:HB3 | 2.00 | 0.42 |
| 13:YA:327[C]:VAL:O | 13:YA:331[C]:ILE:HG22 | 2.20 | 0.42 |
| 13:YA:439[B]:TYR:HB3 | 13:YA:441[B]:ILE:CD1 | 2.50 | 0.42 |
| 13:YA:530[A]:VAL:O | 13:YC:538[A]:VAL:HA | 2.19 | 0.42 |
| 13:YA:538[B]:VAL:O | 13:YC:546[B]:VAL:HA | 2.19 | 0.42 |
| 13:YB:180[C]:LEU:HA | 13:YB:180[C]:LEU:HD13 | 1.76 | 0.42 |
| 13:YB:24[E]:LEU:HA | 13:YB:24[E]:LEU:HD12 | 1.62 | 0.42 |
| 13:YB:26[B]:ARG:HD3 | 14:YE:259[B]:LEU:HD21 | 2.00 | 0.42 |
| 13:YB:296[A]:LEU:HD12 | 13:YB:296[A]:LEU:HA | 1.85 | 0.42 |
| 13:YB:330[E]:ILE:HD12 | 13:YB:336[E]:LEU:HD12 | 2.01 | 0.42 |
| 13:YB:36[E]:PRO:HB2 | 13:YB:38[E]:GLN:OE1 | 2.18 | 0.42 |
| 13:YB:370[D]:ASN:ND2 | 13:YB:372[D]:SER:HB3 | 2.29 | 0.42 |
| 13:YB:38[E]:GLN:O | 13:YB:46[E]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:560[F]:ILE:O | 13:YB:553[F]:LYS:HA | 2.18 | 0.42 |
| 13:YB:66[C]:MET:HE3 | 13:YB:66[C]:MET:HA | 2.00 | 0.42 |
| 13:YB:76[D]:PRO:HG3 | 13:YB:96[D]:VAL:CG1 | 2.48 | 0.42 |
| 13:YC:127[D]:ASN:ND2 | 13:YC:129[D]:THR:OG1 | 2.53 | 0.42 |
| 13:YC:195[C]:GLU:HG2 | 13:YC:197[C]:TYR:CE2 | 2.54 | 0.42 |
| 13:YC:280[F]:MET:O | 13:YC:284[F]:MET:HG2 | 2.20 | 0.42 |
| 13:YC:320[E]:THR:HG22 | 13:YC:323[E]:ARG:HB3 | 2.01 | 0.42 |
| 13:YC:327[F]:VAL:O | 13:YC:331[F]:ILE:HG22 | 2.20 | 0.42 |
| 13:YC:373[F]:ARG:HA | 13:YC:373[F]:ARG:NE | 2.30 | 0.42 |
| 13:YC:389[E]:TYR:O | 13:YC:405[E]:ASP:HB2 | 2.19 | 0.42 |
| 13:YC:454[E]:LYS:C | 13:YC:455[E]:LYS:HG3 | 2.39 | 0.42 |
| 13:YB:476[E]:GLY:HA3 | 13:YC:469[E]:ASN:HA | 2.00 | 0.42 |
| 13:YA:538[D]:VAL:O | 13:YC:546[D]:VAL:HA | 2.19 | 0.42 |
| 13:YC:552[E]:GLU:CG | 13:YC:554[E]:MET:HE1 | 2.49 | 0.42 |
| 14:YD:170[B]:LEU:HD23 | 14:YD:170[B]:LEU:HA | 1.69 | 0.42 |
| 14:YD:17[D]:PHE:HE2 | 14:YD:26[D]:ASN:HA | 1.84 | 0.42 |
| 14:YD:86[E]:ARG:HD2 | 14:YD:192[E]:ILE:HD12 | 2.01 | 0.42 |
| 14:YD:301[E]:MET:O | 14:YD:304[E]:TYR:N | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:238[B]:THR:N | 14:YD:307[B]:TYR:O | 2.53 | 0.42 |
| 14:YD:364[D]:LEU:HA | 14:YD:364[D]:LEU:HD22 | 1.79 | 0.42 |
| 14:YD:373[E]:LYS:HB3 | 14:YD:373[E]:LYS:HE2 | 1.87 | 0.42 |
| 14:YE:114[D]:SER:HA | 14:YE:167[D]:GLU:OE1 | 2.19 | 0.42 |
| 14:YE:114[E]:SER:HA | 14:YE:167[E]:GLU:OE1 | 2.19 | 0.42 |
| 14:YE:172[D]:TYR:CZ | 14:YE:176[D]:VAL:HG21 | 2.54 | 0.42 |
| 14:YE:43[F]:SER:O | 14:YE:189[F]:TRP:HB2 | 2.20 | 0.42 |
| 11:V:178:ASN:HB3 | 14:YE:217[E]:SER:H | 1.83 | 0.42 |
| 13:YB:24[A]:LEU:HD23 | 14:YE:259[A]:LEU:CD2 | 2.49 | 0.42 |
| 14:YE:238[E]:THR:N | 14:YE:307[E]:TYR:O | 2.53 | 0.42 |
| 14:YE:238[F]:THR:N | 14:YE:307[F]:TYR:O | 2.53 | 0.42 |
| 14:YF:238[D]:THR:N | 14:YF:307[D]:TYR:O | 2.53 | 0.42 |
| 14:YF:38[A]:LEU:HA | 14:YF:38[A]:LEU:HD12 | 1.63 | 0.42 |
| 14:YF:75[B]:ALA:HB2 | 14:YF:83[B]:VAL:HA | 2.01 | 0.42 |
| 14:YF:88[E]:TYR:HD1 | 14:YF:110[E]:GLY:C | 2.21 | 0.42 |
| 2:Z:584:GLY:CA | 2:Z:600:PHE:HB3 | 2.48 | 0.42 |
| 2:Z:701:TRP:CG | 2:Z:701:TRP:O | 2.72 | 0.42 |
| 1:A:523:VAL:O | 1:A:531:GLU:HB2 | 2.18 | 0.42 |
| 1:A:559:ALA:N | 1:A:586:ARG:HD2 | 2.33 | 0.42 |
| 5:AC:265:LEU:HD22 | 5:AC:281:TYR:HD2 | 1.84 | 0.42 |
| 5:AD:257:SER:O | 5:AD:258:TYR:HB3 | 2.20 | 0.42 |
| 5:AE:130:PHE:HD2 | 5:AE:152:ASP:HB2 | 1.83 | 0.42 |
| 5:AE:177:PHE:CD2 | 5:AE:230:ILE:HD11 | 2.48 | 0.42 |
| 6:AG:90:PHE:O | 6:AG:154:SER:HB2 | 2.19 | 0.42 |
| 6:AG:82:VAL:HG23 | 6:AG:187:LYS:HE3 | 2.02 | 0.42 |
| 6:AG:195:LEU:HD13 | 6:AG:215:PHE:CE1 | 2.52 | 0.42 |
| 6:AF:12:SER:HB2 | 6:AH:6:ASN:HB3 | 2.00 | 0.42 |
| 7:AI:424:ARG:O | 7:AJ:504:ARG:NH2 | 2.50 | 0.42 |
| 7:AI:429:CYS:HA | 7:BA:511:GLU:OE1 | 2.20 | 0.42 |
| 7:AJ:20:PRO:HB3 | 7:AJ:29:ILE:HG13 | 2.01 | 0.42 |
| 7:AJ:40:SER:HB3 | 7:BA:24:ASN:CB | 2.47 | 0.42 |
| 7:AI:513:ARG:N | 7:AJ:441:GLN:O | 2.34 | 0.42 |
| 7:AJ:451:PHE:HD1 | 7:AJ:469:VAL:HG13 | 1.84 | 0.42 |
| 7:AJ:71:ASN:HB2 | 7:DD:365:GLY:CA | 2.48 | 0.42 |
| 1:B:596:ASN:N | 1:B:596:ASN:OD1 | 2.53 | 0.42 |
| 7:AI:39:ILE:HG22 | 7:BA:44:VAL:CG2 | 2.49 | 0.42 |
| 7:AJ:477:TRP:CZ3 | 7:BA:469:VAL:HB | 2.53 | 0.42 |
| 7:BA:47:VAL:HG12 | 7:BA:48:PRO:N | 2.34 | 0.42 |
| 12:BG:118:TYR:CG | 12:BG:119:ASN:N | 2.86 | 0.42 |
| 1:BH:278:ALA:H | 1:BH:316:GLY:HA2 | 1.85 | 0.42 |
| 1:BH:337:GLN:O | 1:BH:348:PHE:HZ | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:508:ARG:HH22 | 1:BH:577:PHE:HA | 1.84 | 0.42 |
| 1:BI:307:ASP:OD1 | 1:BI:307:ASP:N | 2.53 | 0.42 |
| 1:BI:378:PRO:O | 1:BI:379:LYS:HG2 | 2.19 | 0.42 |
| 2:BJ:572:ASN:CB | 2:BJ:611:ILE:HG22 | 2.48 | 0.42 |
| 2:BJ:701:TRP:CG | 2:BJ:701:TRP:O | 2.72 | 0.42 |
| 2:C:186:ASP:HB3 | 2:C:189:ARG:CD | 2.49 | 0.42 |
| 2:C:761:GLU:HB2 | 2:C:862:TYR:CE1 | 2.54 | 0.42 |
| 2:C:981:GLN:CG | 2:C:982:LEU:N | 2.82 | 0.42 |
| 3:CA:254:ASP:HB3 | 3:CA:257:TYR:HD2 | 1.84 | 0.42 |
| 3:CB:228:ASN:HA | 3:CB:229:LEU:HD13 | 2.01 | 0.42 |
| 4:CD:131:LYS:HD3 | 4:CD:161:ASN:HD22 | 1.85 | 0.42 |
| 5:CF:134:GLU:O | 5:CF:145:TYR:HA | 2.19 | 0.42 |
| 5:CF:304:ILE:HG21 | 5:CF:309:LEU:HD12 | 2.01 | 0.42 |
| 5:CF:321:ALA:O | 5:CF:324:VAL:HG12 | 2.19 | 0.42 |
| 5:CF:407:TYR:CD1 | 5:CH:407:TYR:HB2 | 2.54 | 0.42 |
| 5:CF:477:SER:O | 5:CF:601:ILE:N | 2.50 | 0.42 |
| 5:CG:49:TRP:N | 5:CG:49:TRP:CD1 | 2.87 | 0.42 |
| 5:CH:137:TYR:HD1 | 5:CH:143:TRP:HE1 | 1.61 | 0.42 |
| 5:CH:196:ARG:HH22 | 7:DC:9:VAL:HG13 | 1.84 | 0.42 |
| 5:CH:186:TYR:O | 5:CH:227:GLY:HA3 | 2.20 | 0.42 |
| 5:CH:304:ILE:HD12 | 5:CH:306:PRO:HA | 2.02 | 0.42 |
| 5:CH:322:GLY:CA | 5:CH:359:GLU:HA | 2.50 | 0.42 |
| 6:CI:201:VAL:N | 6:CI:210:THR:O | 2.31 | 0.42 |
| 2:C:915:LYS:HG2 | 3:D:326:GLU:OE2 | 2.20 | 0.42 |
| 7:DB:163:LEU:HD23 | 7:DB:167:GLN:HB2 | 2.01 | 0.42 |
| 7:DB:183:ALA:O | 7:DB:187:ASP:HB2 | 2.19 | 0.42 |
| 7:DB:96:GLY:H | 7:DD:98:THR:H | 1.67 | 0.42 |
| 7:DC:491:ASP:HB2 | 7:DC:496:ARG:HG2 | 2.01 | 0.42 |
| 7:DD:445:HIS:CD2 | 7:DD:447:HIS:CE1 | 3.06 | 0.42 |
| 8:DE:18:PRO:HD3 | 8:FH:151:GLN:N | 2.34 | 0.42 |
| 10:DH:133:LYS:HB3 | 10:DH:208:THR:O | 2.19 | 0.42 |
| 11:DI:107:ASP:HA | 11:DI:155:THR:HG22 | 2.00 | 0.42 |
| 3:E:79:VAL:HG12 | 3:E:80:LYS:O | 2.18 | 0.42 |
| 1:EA:392:ILE:HG23 | 1:EA:408:ILE:HD12 | 2.01 | 0.42 |
| 1:EB:378:PRO:O | 1:EB:379:LYS:HG2 | 2.19 | 0.42 |
| 2:EC:480:LEU:CD2 | 2:EC:488:MET:HB2 | 2.49 | 0.42 |
| 3:ED:237:GLY:O | 3:ED:240:TYR:N | 2.48 | 0.42 |
| 2:EC:915:LYS:HG2 | 3:ED:326:GLU:OE2 | 2.20 | 0.42 |
| 4:EF:17:ASN:OD1 | 4:EF:18:ALA:N | 2.53 | 0.42 |
| 4:EG:43:GLY:HA2 | 4:EG:62:HIS:CE1 | 2.55 | 0.42 |
| 4:EG:44:ASP:O | 4:EG:59:GLN:NE2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:89:TYR:CD1 | 5:EI:139:ALA:HA | 2.53 | 0.42 |
| 5:EI:134:GLU:O | 5:EI:145:TYR:HA | 2.19 | 0.42 |
| 5:EI:323:THR:CG2 | 5:EI:354:THR:HG23 | 2.48 | 0.42 |
| 5:EJ:150:GLN:C | 5:EJ:151:ILE:HG13 | 2.40 | 0.42 |
| 5:EJ:389:ASP:OD1 | 5:EJ:389:ASP:N | 2.51 | 0.42 |
| 5:EJ:395:THR:OG1 | 5:EJ:396:LYS:N | 2.52 | 0.42 |
| 5:EJ:34:TYR:OH | 5:EJ:41:ASP:C | 2.58 | 0.42 |
| 5:FA:357:SER:HA | 5:FA:371:PHE:CD1 | 2.54 | 0.42 |
| 5:FA:371:PHE:HZ | 5:FA:373:SER:HB3 | 1.84 | 0.42 |
| 5:FA:491:ASN:OD1 | 5:FA:493:ASP:N | 2.48 | 0.42 |
| 5:EI:548:GLY:O | 5:FA:568:LYS:HB3 | 2.18 | 0.42 |
| 5:FA:340:VAL:HG21 | 6:FB:174:TYR:H | 1.83 | 0.42 |
| 6:FB:195:LEU:HD13 | 6:FB:215:PHE:CE1 | 2.52 | 0.42 |
| 6:FC:47:PHE:HE2 | 6:FC:51:ASN:HB3 | 1.84 | 0.42 |
| 6:FD:11:ILE:HB | 6:FD:12:SER:H | 1.66 | 0.42 |
| 6:FD:90:PHE:O | 6:FD:154:SER:HB2 | 2.19 | 0.42 |
| 7:FE:251:ASN:HB2 | 7:FF:253:ARG:HH22 | 1.83 | 0.42 |
| 7:FE:466:SER:HB3 | 7:FE:468:PHE:CE2 | 2.54 | 0.42 |
| 7:FF:20:PRO:HB3 | 7:FF:29:ILE:HG13 | 2.01 | 0.42 |
| 7:FF:267:THR:O | 7:FF:285:ALA:HA | 2.19 | 0.42 |
| 7:FF:354:LEU:HD21 | 7:FF:522:ILE:HG21 | 2.00 | 0.42 |
| 7:FF:85:LEU:C | 7:FF:88:PRO:HD3 | 2.40 | 0.42 |
| 7:FE:301:ARG:O | 7:FG:295:ILE:HA | 2.19 | 0.42 |
| 8:FI:21:PHE:CG | 8:IB:142:LEU:HD21 | 2.54 | 0.42 |
| 8:FI:25:ILE:O | 8:FI:26:SER:HB3 | 2.19 | 0.42 |
| 9:FJ:85:GLU:OE2 | 9:FJ:87:ARG:NH2 | 2.53 | 0.42 |
| 4:F:168:PHE:CE1 | 4:G:161:ASN:HB3 | 2.54 | 0.42 |
| 12:GC:99:SER:HB3 | 12:GC:102:GLY:H | 1.84 | 0.42 |
| 12:GC:140:ASP:OD1 | 12:GC:141:TRP:N | 2.52 | 0.42 |
| 1:GD:494:THR:HG22 | 1:GD:498:GLY:HA2 | 2.01 | 0.42 |
| 1:GD:592:ILE:O | 1:GD:608:LYS:HD2 | 2.19 | 0.42 |
| 1:GE:654:ASP:OD1 | 1:GE:655:LEU:N | 2.52 | 0.42 |
| 3:EE:265:GLY:HA3 | 1:GE:656:GLU:OE2 | 2.19 | 0.42 |
| 2:GF:1005:ARG:NH1 | 5:HB:12:ASP:OD2 | 2.52 | 0.42 |
| 2:GF:321:VAL:HA | 2:GF:326:VAL:HA | 2.01 | 0.42 |
| 2:GF:380:ILE:HB | 2:GF:396:ILE:HG21 | 2.01 | 0.42 |
| 1:B:390:GLU:HG2 | 2:GF:603:ARG:HH12 | 1.85 | 0.42 |
| 2:EC:450:PHE:HE2 | 3:GG:70:ASP:OD2 | 2.01 | 0.42 |
| 4:GI:17:ASN:OD1 | 4:GI:18:ALA:N | 2.53 | 0.42 |
| 4:GJ:100:ARG:NH2 | 4:GJ:128:ASP:OD1 | 2.53 | 0.42 |
| 4:GJ:124:ILE:HB | 4:GJ:137:LEU:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:GJ:251:ASN:N | 4:GJ:266:SER:O | 2.53 | 0.42 |
| 4:H:251:ASN:N | 4:H:266:SER:O | 2.53 | 0.42 |
| 5:HB:304:ILE:HG21 | 5:HB:309:LEU:HD12 | 2.01 | 0.42 |
| 5:HB:322:GLY:HA2 | 5:HB:360:THR:N | 2.34 | 0.42 |
| 5:HC:68:TYR:HB2 | 5:HC:70:ILE:HD11 | 2.00 | 0.42 |
| 5:HD:357:SER:HB3 | 5:HD:358:VAL:H | 1.55 | 0.42 |
| 6:HE:108:LEU:HD23 | 6:HE:113:PRO:HA | 2.00 | 0.42 |
| 6:HE:217:ARG:HE | 6:HE:219:ALA:C | 2.23 | 0.42 |
| 6:HE:164:GLN:NE2 | 6:HG:57:ASN:HB2 | 2.34 | 0.42 |
| 7:HH:444:TYR:HB2 | 7:HJ:486:ASP:HB2 | 2.01 | 0.42 |
| 7:HI:267:THR:O | 7:HI:285:ALA:HA | 2.19 | 0.42 |
| 7:HI:75:ALA:HB1 | 7:HJ:75:ALA:HB1 | 2.02 | 0.42 |
| 7:HJ:20:PRO:CD | 7:HJ:29:ILE:HG21 | 2.49 | 0.42 |
| 5:I:272:SER:OG | 6:L:106:THR:N | 2.52 | 0.42 |
| 5:I:572:ALA:HA | 5:J:540:GLU:HG2 | 2.02 | 0.42 |
| 12:W:99:SER:HB2 | 12:IF:215:MET:CE | 2.49 | 0.42 |
| 5:J:290:SER:HA | 5:J:371:PHE:H | 1.85 | 0.42 |
| 5:J:341:GLU:C | 5:J:343:SER:H | 2.22 | 0.42 |
| 5:K:196:ARG:HH22 | 7:P:9:VAL:HG13 | 1.85 | 0.42 |
| 5:I:196:ARG:O | 5:K:197:GLY:HA2 | 2.19 | 0.42 |
| 5:K:290:SER:HB3 | 5:K:370:HIS:HA | 2.02 | 0.42 |
| 6:L:57:ASN:HB2 | 6:M:164:GLN:NE2 | 2.34 | 0.42 |
| 6:M:44:ALA:HA | 6:N:110:PHE:C | 2.40 | 0.42 |
| 5:J:339:GLU:HB3 | 6:N:172:SER:O | 2.20 | 0.42 |
| 7:O:77:THR:CG2 | 7:O:80:THR:H | 2.33 | 0.42 |
| 7:P:85:LEU:C | 7:P:88:PRO:HD3 | 2.40 | 0.42 |
| 7:Q:111:ASN:ND2 | 7:Q:114:SER:HB3 | 2.34 | 0.42 |
| 8:R:25:ILE:O | 8:R:26:SER:HB3 | 2.19 | 0.42 |
| 8:S:25:ILE:O | 8:S:26:SER:HB3 | 2.20 | 0.42 |
| 1:X:559:ALA:N | 1:X:586:ARG:HD2 | 2.33 | 0.42 |
| 1:Y:174:ARG:HA | 1:Y:270:ILE:O | 2.19 | 0.42 |
| 1:Y:209:TRP:CZ3 | 1:Y:212:LYS:NZ | 2.69 | 0.42 |
| 1:Y:213:SER:HA | 2:Z:733:ASP:CG | 2.40 | 0.42 |
| 1:Y:611:LEU:HD11 | 1:Y:616:PHE:CE2 | 2.54 | 0.42 |
| 13:YA:132[E]:LEU:O | 13:YA:390[E]:VAL:HG11 | 2.19 | 0.42 |
| 13:YA:147[F]:ILE:HD11 | 13:YA:188[F]:LEU:HG | 2.00 | 0.42 |
| 13:YA:195[E]:GLU:HG2 | 13:YA:197[E]:TYR:CE2 | 2.54 | 0.42 |
| 13:YA:304[F]:TRP:O | 13:YA:308[F]:TYR:N | 2.33 | 0.42 |
| 13:YA:327[F]:VAL:O | 13:YA:331[F]:ILE:HG22 | 2.20 | 0.42 |
| 13:YA:538[F]:VAL:O | 13:YC:546[F]:VAL:HA | 2.19 | 0.42 |
| 13:YA:66[D]:MET:HE3 | 13:YA:66[D]:MET:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:127[D]:ASN:ND2 | 13:YB:129[D]:THR:OG1 | 2.53 | 0.42 |
| 13:YB:195[C]:GLU:HG2 | 13:YB:197[C]:TYR:CE2 | 2.54 | 0.42 |
| 13:YB:195[E]:GLU:HG2 | 13:YB:197[E]:TYR:CE2 | 2.54 | 0.42 |
| 13:YB:200[D]:ILE:HD13 | 13:YB:236[D]:ILE:HD12 | 2.01 | 0.42 |
| 13:YB:280[C]:MET:O | 13:YB:284[C]:MET:HG2 | 2.20 | 0.42 |
| 13:YB:280[D]:MET:O | 13:YB:284[D]:MET:HG2 | 2.19 | 0.42 |
| 13:YB:38[D]:GLN:O | 13:YB:46[D]:GLY:HA2 | 2.20 | 0.42 |
| 13:YB:38[F]:GLN:O | 13:YB:46[F]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:70[A]:GLY:O | 13:YB:394[A]:GLU:N | 2.52 | 0.42 |
| 13:YB:442[B]:THR:HB | 13:YC:434[B]:THR:HB | 2.01 | 0.42 |
| 13:YB:66[A]:MET:HE3 | 13:YB:66[A]:MET:HA | 2.00 | 0.42 |
| 13:YC:187[C]:ARG:HD3 | 13:YC:187[C]:ARG:HA | 1.87 | 0.42 |
| 13:YC:277[D]:LEU:HA | 13:YC:277[D]:LEU:HD23 | 1.80 | 0.42 |
| 13:YC:330[B]:ILE:HD12 | 13:YC:336[B]:LEU:HD12 | 2.01 | 0.42 |
| 13:YC:132[C]:LEU:O | 13:YC:390[C]:VAL:HG11 | 2.19 | 0.42 |
| 13:YC:564[A]:GLN:HG3 | 13:YC:566[A]:THR:HG22 | 2.01 | 0.42 |
| 10:BE:287:VAL:O | 14:YD:100[E]:LYS:HD3 | 2.19 | 0.42 |
| 14:YD:112[B]:ILE:HB | 14:YD:140[B]:TYR:OH | 2.20 | 0.42 |
| 14:YD:86[F]:ARG:HD2 | 14:YD:192[F]:ILE:HD12 | 2.02 | 0.42 |
| 14:YD:238[A]:THR:N | 14:YD:307[A]:TYR:O | 2.53 | 0.42 |
| 14:YE:86[F]:ARG:HD2 | 14:YE:192[F]:ILE:HD12 | 2.02 | 0.42 |
| 14:YE:330[B]:LYS:HG2 | 14:YF:101[B]:GLY:HA3 | 2.00 | 0.42 |
| 14:YE:86[C]:ARG:HD2 | 14:YE:192[C]:ILE:HD12 | 2.01 | 0.42 |
| 14:YD:242[A]:PRO:HD2 | 14:YE:91[A]:LYS:O | 2.19 | 0.42 |
| 14:YD:242[F]:PRO:HD2 | 14:YE:91[F]:LYS:O | 2.19 | 0.42 |
| 14:YF:86[A]:ARG:HD2 | 14:YF:192[A]:ILE:HD12 | 2.01 | 0.42 |
| 14:YF:290[C]:ASN:C | 14:YF:290[C]:ASN:OD1 | 2.58 | 0.42 |
| 14:YF:301[A]:MET:O | 14:YF:304[A]:TYR:N | 2.49 | 0.42 |
| 2:Z:439:LYS:HG3 | 2:Z:440:LEU:HD12 | 2.02 | 0.42 |
| 2:Z:139:ASN:HA | 2:Z:555:ARG:NH2 | 2.34 | 0.42 |
| 1:A:192:ILE:HG22 | 1:A:272:TYR:CD1 | 2.54 | 0.42 |
| 1:A:90:VAL:HG11 | 1:A:228:GLU:HG2 | 2.01 | 0.42 |
| 4:AA:131:LYS:HD3 | 4:AA:161:ASN:HD22 | 1.85 | 0.42 |
| 4:AB:190:PRO:HA | 4:AB:262:THR:HA | 2.01 | 0.42 |
| 5:AC:261:ARG:HB2 | 5:AC:383:ILE:HB | 2.01 | 0.42 |
| 5:AC:304:ILE:HG12 | 5:AC:305:ASN:O | 2.20 | 0.42 |
| 5:AC:36:GLU:OE1 | 5:AC:66:LYS:HG2 | 2.19 | 0.42 |
| 5:AC:477:SER:O | 5:AC:601:ILE:N | 2.50 | 0.42 |
| 5:AD:102:TRP:N | 5:AD:102:TRP:CD1 | 2.86 | 0.42 |
| 5:AD:129:ARG:HG3 | 5:AD:130:PHE:N | 2.33 | 0.42 |
| 5:AD:316:ILE:HD13 | 6:AF:7:LYS:HG3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AD:303:PRO:HD2 | 5:AD:365:ILE:HD13 | 2.02 | 0.42 |
| 5:AD:290:SER:CA | 5:AD:371:PHE:H | 2.33 | 0.42 |
| 5:AE:304:ILE:HD12 | 5:AE:304:ILE:O | 2.20 | 0.42 |
| 6:AF:90:PHE:O | 6:AF:154:SER:HB2 | 2.19 | 0.42 |
| 6:AF:64:ILE:HG23 | 6:AF:217:ARG:HH12 | 1.84 | 0.42 |
| 6:AH:47:PHE:HE2 | 6:AH:51:ASN:HB3 | 1.84 | 0.42 |
| 7:AI:212:PRO:CB | 7:AJ:199:VAL:HA | 2.49 | 0.42 |
| 7:AJ:77:THR:OG1 | 7:AJ:78:PRO:HD2 | 2.19 | 0.42 |
| 1:B:209:TRP:O | 1:B:210:THR:C | 2.58 | 0.42 |
| 1:A:227:ARG:HH21 | 1:B:81:ARG:NH2 | 2.18 | 0.42 |
| 7:AJ:212:PRO:CB | 7:BA:199:VAL:HA | 2.43 | 0.42 |
| 7:BA:445:HIS:CD2 | 7:BA:447:HIS:CE1 | 3.06 | 0.42 |
| 10:BE:322:ASP:O | 10:BE:342:PHE:HB2 | 2.19 | 0.42 |
| 11:BF:186:ARG:HG3 | 11:BF:187:ILE:N | 2.33 | 0.42 |
| 11:BF:88:THR:O | 11:BF:163:ASN:ND2 | 2.53 | 0.42 |
| 12:BG:99:SER:HB3 | 12:BG:102:GLY:H | 1.84 | 0.42 |
| 1:BI:158:ASN:CG | 1:BI:160:GLN:HG2 | 2.40 | 0.42 |
| 1:BI:533:ASP:O | 1:BI:535:LEU:N | 2.53 | 0.42 |
| 2:BJ:669:GLU:O | 2:BJ:672:ILE:N | 2.52 | 0.42 |
| 2:BJ:73:ASP:HB3 | 2:BJ:76:THR:HG21 | 2.02 | 0.42 |
| 2:BJ:750:VAL:HG23 | 2:BJ:751:LEU:H | 1.84 | 0.42 |
| 2:BJ:937:THR:HA | 2:BJ:941:GLU:O | 2.19 | 0.42 |
| 2:BJ:980:GLY:C | 2:BJ:983:PRO:HD2 | 2.40 | 0.42 |
| 2:C:1019:PRO:HG3 | 3:D:93:ARG:HD3 | 2.01 | 0.42 |
| 2:C:541:TYR:CG | 2:C:542:THR:N | 2.85 | 0.42 |
| 2:C:750:VAL:HG23 | 2:C:751:LEU:H | 1.84 | 0.42 |
| 4:CC:100:ARG:NH2 | 4:CC:128:ASP:OD1 | 2.53 | 0.42 |
| 4:CC:131:LYS:HD3 | 4:CC:161:ASN:HD22 | 1.85 | 0.42 |
| 4:CD:61:ILE:O | 4:CE:4:GLN:NE2 | 2.50 | 0.42 |
| 4:CE:17:ASN:OD1 | 4:CE:18:ALA:N | 2.53 | 0.42 |
| 4:CE:43:GLY:HA2 | 4:CE:62:HIS:CE1 | 2.55 | 0.42 |
| 5:CG:102:TRP:CD1 | 5:CG:102:TRP:N | 2.86 | 0.42 |
| 2:BJ:220:LYS:HA | 5:CG:562:SER:OG | 2.19 | 0.42 |
| 5:CH:186:TYR:HB3 | 5:CH:227:GLY:C | 2.39 | 0.42 |
| 5:CH:532:LEU:HA | 5:CH:532:LEU:HD23 | 1.87 | 0.42 |
| 5:CH:58:GLN:OE1 | 5:CH:58:GLN:N | 2.37 | 0.42 |
| 5:CH:89:TYR:C | 5:CH:91:LYS:H | 2.23 | 0.42 |
| 6:CI:57:ASN:HB2 | 6:CJ:164:GLN:NE2 | 2.34 | 0.42 |
| 7:DB:228:ILE:HG21 | 7:DB:244:ALA:HB2 | 2.01 | 0.42 |
| 7:DB:378:ARG:NH1 | 7:DD:355:PRO:HG3 | 2.34 | 0.42 |
| 7:DD:101:SER:OG | 7:DD:102:THR:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DD:26:PRO:HA | 7:DD:27:PRO:HD3 | 1.69 | 0.42 |
| 7:DB:473:LYS:CD | 7:DD:473:LYS:HB3 | 2.41 | 0.42 |
| 7:DD:47:VAL:HG12 | 7:DD:48:PRO:N | 2.34 | 0.42 |
| 7:DB:444:TYR:HB2 | 7:DD:486:ASP:HB2 | 2.01 | 0.42 |
| 9:DG:64:ASN:O | 9:DG:69:THR:HG21 | 2.19 | 0.42 |
| 1:EA:192:ILE:HG22 | 1:EA:272:TYR:CE1 | 2.54 | 0.42 |
| 2:EC:1019:PRO:HG3 | 3:ED:93:ARG:HD3 | 2.01 | 0.42 |
| 2:EC:855:ILE:HA | 2:EC:855:ILE:HD12 | 1.86 | 0.42 |
| 4:EG:224:ASP:OD2 | 4:EG:227:ASN:HB2 | 2.19 | 0.42 |
| 4:EH:43:GLY:HA2 | 4:EH:62:HIS:CE1 | 2.55 | 0.42 |
| 5:EI:170:GLU:O | 5:EI:171:VAL:HG12 | 2.19 | 0.42 |
| 5:EI:549:SER:N | 5:FA:569:TYR:O | 2.53 | 0.42 |
| 4:F:17:ASN:OD1 | 4:F:18:ALA:N | 2.53 | 0.42 |
| 5:EI:41:ASP:HB3 | 5:FA:1:MET:H3 | 1.85 | 0.42 |
| 5:FA:215:PRO:HB3 | 5:FA:229:ASN:O | 2.19 | 0.42 |
| 5:EI:30:PHE:CE1 | 5:FA:30:PHE:CE1 | 3.05 | 0.42 |
| 5:FA:89:TYR:C | 5:FA:91:LYS:H | 2.23 | 0.42 |
| 6:FB:217:ARG:HE | 6:FB:219:ALA:C | 2.23 | 0.42 |
| 6:FC:217:ARG:HE | 6:FC:219:ALA:C | 2.23 | 0.42 |
| 7:FE:197:ALA:O | 7:FE:201:GLN:HG3 | 2.20 | 0.42 |
| 7:FF:146:SER:HB2 | 7:FF:149:GLN:HG2 | 2.01 | 0.42 |
| 7:FF:77:THR:OG1 | 7:FF:78:PRO:HD2 | 2.19 | 0.42 |
| 7:FG:134:SER:N | 7:FG:142:ILE:HD11 | 2.35 | 0.42 |
| 7:FE:473:LYS:CD | 7:FG:473:LYS:HB3 | 2.43 | 0.42 |
| 4:G:190:PRO:HA | 4:G:262:THR:HA | 2.01 | 0.42 |
| 11:GB:88:THR:O | 11:GB:163:ASN:ND2 | 2.53 | 0.42 |
| 11:GB:178:ASN:HB3 | 14:YD:217[E]:SER:H | 1.85 | 0.42 |
| 1:GD:146:VAL:HG11 | 1:GD:172:ILE:HG12 | 2.01 | 0.42 |
| 1:GD:209:TRP:CD1 | 1:GD:225:TYR:HE1 | 2.34 | 0.42 |
| 1:GD:306:ASP:N | 1:GD:306:ASP:OD1 | 2.52 | 0.42 |
| 2:GF:114:ILE:HG23 | 2:GF:115:GLU:H | 1.83 | 0.42 |
| 2:GF:135:VAL:HG12 | 2:GF:589:LYS:HE3 | 2.01 | 0.42 |
| 2:GF:644:ASP:HB2 | 2:GF:646:ARG:HG2 | 2.01 | 0.42 |
| 2:GF:761:GLU:HB2 | 2:GF:862:TYR:CE1 | 2.54 | 0.42 |
| 2:GF:980:GLY:C | 2:GF:983:PRO:HD2 | 2.40 | 0.42 |
| 4:GI:131:LYS:HD3 | 4:GI:161:ASN:HD22 | 1.85 | 0.42 |
| 4:GI:145:LYS:N | 4:GI:165:GLU:O | 2.49 | 0.42 |
| 4:GI:63:ALA:HB3 | 4:GJ:83:THR:HA | 2.02 | 0.42 |
| 4:H:131:LYS:HD3 | 4:H:161:ASN:HD22 | 1.85 | 0.42 |
| 4:H:190:PRO:HA | 4:H:262:THR:HA | 2.01 | 0.42 |
| 4:H:209:VAL:HG13 | 4:H:271:GLY:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:44:ASP:O | 4:H:59:GLN:NE2 | 2.52 | 0.42 |
| 4:HA:43:GLY:HA2 | 4:HA:62:HIS:CE1 | 2.55 | 0.42 |
| 5:HB:49:TRP:HZ3 | 5:HB:96:ARG:HD2 | 1.80 | 0.42 |
| 5:HC:139:ALA:HB3 | 5:HC:140:PRO:HD3 | 2.01 | 0.42 |
| 5:HD:368:ILE:HG13 | 5:HD:369:LEU:N | 2.35 | 0.42 |
| 5:HD:497:PRO:HG2 | 5:HD:498:ASN:ND2 | 2.35 | 0.42 |
| 7:HH:228:ILE:HG21 | 7:HH:244:ALA:HB2 | 2.01 | 0.42 |
| 7:HH:375:TYR:CE2 | 7:HH:390:PRO:HB2 | 2.53 | 0.42 |
| 7:HI:99:ARG:HH11 | 7:HI:111:ASN:ND2 | 2.18 | 0.42 |
| 7:HJ:196:VAL:HG22 | 7:HJ:214:THR:HG22 | 2.02 | 0.42 |
| 5:I:107:VAL:HB | 5:I:126:ILE:HB | 2.01 | 0.42 |
| 5:I:36:GLU:OE1 | 5:I:66:LYS:HG2 | 2.19 | 0.42 |
| 5:J:257:SER:O | 5:J:258:TYR:HB3 | 2.20 | 0.42 |
| 5:K:89:TYR:C | 5:K:91:LYS:H | 2.23 | 0.42 |
| 7:O:466:SER:HB3 | 7:O:468:PHE:CE2 | 2.54 | 0.42 |
| 7:O:78:PRO:HB2 | 7:P:69:GLY:HA2 | 2.02 | 0.42 |
| 7:Q:134:SER:N | 7:Q:142:ILE:HD11 | 2.35 | 0.42 |
| 7:O:188:GLN:NE2 | 7:Q:192:GLN:OE1 | 2.53 | 0.42 |
| 8:R:15:PHE:N | 8:R:15:PHE:CD1 | 2.84 | 0.42 |
| 12:W:192:PRO:O | 12:W:219:HIS:NE2 | 2.52 | 0.42 |
| 1:X:361:GLN:HE21 | 1:X:456:ASN:HB2 | 1.84 | 0.42 |
| 1:X:377:LYS:HD3 | 1:X:641:VAL:HG21 | 2.02 | 0.42 |
| 13:YA:127[D]:ASN:ND2 | 13:YA:129[D]:THR:OG1 | 2.53 | 0.42 |
| 13:YA:127[A]:ASN:ND2 | 13:YA:129[A]:THR:OG1 | 2.53 | 0.42 |
| 13:YA:320[E]:THR:HG22 | 13:YA:323[E]:ARG:HB3 | 2.00 | 0.42 |
| 13:YA:439[F]:TYR:HB3 | 13:YA:441[F]:ILE:CD1 | 2.49 | 0.42 |
| 13:YA:452[A]:GLY:O | 13:YC:460[A]:GLY:N | 2.50 | 0.42 |
| 13:YA:454[C]:LYS:C | 13:YA:455[C]:LYS:HG3 | 2.40 | 0.42 |
| 13:YA:38[F]:GLN:O | 13:YA:46[F]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:550[B]:TRP:HB2 | 13:YC:554[B]:MET:HG3 | 2.02 | 0.42 |
| 13:YA:66[F]:MET:HA | 13:YA:66[F]:MET:HE3 | 2.01 | 0.42 |
| 13:YA:83[A]:TYR:OH | 13:YA:85[A]:HIS:HE1 | 2.03 | 0.42 |
| 13:YB:293[B]:ASN:HA | 13:YB:296[B]:LEU:HB2 | 2.01 | 0.42 |
| 13:YB:439[A]:TYR:HB3 | 13:YB:441[A]:ILE:CD1 | 2.49 | 0.42 |
| 13:YB:515[E]:LYS:HG3 | 13:YC:507[E]:GLU:HA | 2.02 | 0.42 |
| 13:YB:552[F]:GLU:HB2 | 13:YB:554[F]:MET:HE1 | 2.01 | 0.42 |
| 13:YB:566[C]:THR:HG23 | 13:YC:558[C]:SER:HA | 2.01 | 0.42 |
| 13:YB:83[A]:TYR:OH | 13:YB:85[A]:HIS:HE1 | 2.03 | 0.42 |
| 13:YB:83[D]:TYR:OH | 13:YB:85[D]:HIS:HE1 | 2.03 | 0.42 |
| 13:YC:187[D]:ARG:HD3 | 13:YC:187[D]:ARG:HA | 1.87 | 0.42 |
| 13:YA:363[B]:PRO:HB2 | 13:YC:284[B]:MET:HE3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:320[F]:THR:HG22 | 13:YC:323[F]:ARG:HB3 | 2.00 | 0.42 |
| 13:YC:327[C]:VAL:O | 13:YC:331[C]:ILE:HG22 | 2.20 | 0.42 |
| 13:YC:38[B]:GLN:O | 13:YC:46[B]:GLY:HA2 | 2.20 | 0.42 |
| 13:YC:454[C]:LYS:C | 13:YC:455[C]:LYS:HG3 | 2.39 | 0.42 |
| 13:YA:463[E]:ILE:HA | 13:YC:471[E]:LEU:O | 2.20 | 0.42 |
| 13:YB:530[A]:VAL:HG22 | 13:YC:522[A]:VAL:HG13 | 2.01 | 0.42 |
| 14:YD:112[A]:ILE:HB | 14:YD:140[A]:TYR:OH | 2.20 | 0.42 |
| 14:YD:290[A]:ASN:OD1 | 14:YD:290[A]:ASN:C | 2.58 | 0.42 |
| 14:YE:43[E]:SER:O | 14:YE:189[E]:TRP:HB2 | 2.20 | 0.42 |
| 14:YE:86[A]:ARG:HD2 | 14:YE:192[A]:ILE:HD12 | 2.01 | 0.42 |
| 14:YE:334[A]:LYS:HD2 | 14:YE:334[A]:LYS:HA | 1.91 | 0.42 |
| 14:YE:47[D]:ARG:NH1 | 14:YE:341[D]:GLU:OE1 | 2.53 | 0.42 |
| 14:YE:38[C]:LEU:HD12 | 14:YE:38[C]:LEU:HA | 1.63 | 0.42 |
| 14:YD:236[A]:TRP:N | 14:YE:95[A]:VAL:O | 2.52 | 0.42 |
| 14:YF:112[C]:ILE:HB | 14:YF:140[C]:TYR:OH | 2.20 | 0.42 |
| 14:YF:43[E]:SER:O | 14:YF:189[E]:TRP:HB2 | 2.20 | 0.42 |
| 13:YA:81[A]:ARG:HD3 | 14:YF:261[A]:SER:HA | 2.01 | 0.42 |
| 14:YF:75[D]:ALA:HB2 | 14:YF:83[D]:VAL:HA | 2.01 | 0.42 |
| 2:Z:18:ALA:HB2 | 2:Z:103:PHE:O | 2.19 | 0.42 |
| 2:Z:114:ILE:HG23 | 2:Z:115:GLU:H | 1.83 | 0.42 |
| 2:Z:21:VAL:HG23 | 2:Z:69:PHE:HB3 | 2.02 | 0.42 |
| 2:Z:300:LEU:N | 2:Z:301:PRO:HD3 | 2.34 | 0.42 |
| 2:Z:59:LEU:HD23 | 2:Z:59:LEU:HA | 1.85 | 0.42 |
| 2:Z:33:TYR:CE1 | 2:Z:85:ALA:HB3 | 2.55 | 0.42 |
| 1:A:361:GLN:HE21 | 1:A:456:ASN:HB2 | 1.84 | 0.42 |
| 1:A:59:LEU:CD1 | 1:B:37:LEU:HD12 | 2.50 | 0.42 |
| 1:A:609:ILE:HG22 | 1:A:611:LEU:HG | 2.01 | 0.42 |
| 1:A:64:THR:HG21 | 2:C:674:TYR:HE2 | 1.84 | 0.42 |
| 4:AB:17:ASN:OD1 | 4:AB:18:ALA:N | 2.52 | 0.42 |
| 5:AD:169:VAL:HG13 | 5:AD:174:GLN:OE1 | 2.20 | 0.42 |
| 5:AD:288:MET:HE2 | 5:AD:292:PRO:HD3 | 2.01 | 0.42 |
| 5:AE:186:TYR:O | 5:AE:227:GLY:HA3 | 2.20 | 0.42 |
| 5:AE:196:ARG:HH22 | 7:AJ:9:VAL:HG13 | 1.83 | 0.42 |
| 5:AE:311:VAL:HA | 5:AE:382:ASN:O | 2.20 | 0.42 |
| 6:AF:141:THR:HG22 | 6:AH:43:LEU:HD11 | 2.01 | 0.42 |
| 7:AJ:99:ARG:HH11 | 7:AJ:111:ASN:ND2 | 2.17 | 0.42 |
| 7:AJ:46:GLY:O | 7:AJ:47:VAL:HG23 | 2.19 | 0.42 |
| 7:BA:101:SER:OG | 7:BA:102:THR:N | 2.52 | 0.42 |
| 7:AI:435:GLY:HA2 | 7:BA:517:ILE:HD11 | 2.01 | 0.42 |
| 8:BB:25:ILE:O | 8:BB:26:SER:HB3 | 2.20 | 0.42 |
| 8:BC:21:PHE:CG | 8:DF:142:LEU:HD21 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:BE:311:PHE:HB3 | 10:BE:312:GLY:H | 1.44 | 0.42 |
| 1:BH:277:GLY:O | 1:BH:279:ASP:N | 2.50 | 0.42 |
| 1:BH:392:ILE:HG23 | 1:BH:408:ILE:HD12 | 2.01 | 0.42 |
| 1:BI:206:TRP:CG | 1:BI:222:THR:HB | 2.53 | 0.42 |
| 2:BJ:18:ALA:HB2 | 2:BJ:103:PHE:O | 2.19 | 0.42 |
| 2:BJ:314:THR:HG23 | 2:BJ:317:TYR:HB2 | 2.01 | 0.42 |
| 2:BJ:480:LEU:CD2 | 2:BJ:488:MET:HB2 | 2.49 | 0.42 |
| 2:BJ:683:TYR:O | 2:BJ:686:LEU:N | 2.53 | 0.42 |
| 2:C:73:ASP:HB3 | 2:C:76:THR:HG21 | 2.02 | 0.42 |
| 2:C:33:TYR:CE1 | 2:C:85:ALA:HB3 | 2.55 | 0.42 |
| 2:C:967:ASP:N | 2:C:967:ASP:OD1 | 2.53 | 0.42 |
| 4:CD:17:ASN:OD1 | 4:CD:18:ALA:N | 2.53 | 0.42 |
| 5:CF:304:ILE:HG12 | 5:CF:305:ASN:O | 2.20 | 0.42 |
| 5:CF:460:TYR:CE1 | 5:CG:458:THR:HG23 | 2.54 | 0.42 |
| 5:CG:116:THR:HG22 | 5:CG:121:ALA:HB2 | 2.02 | 0.42 |
| 5:CG:150:GLN:C | 5:CG:151:ILE:HG13 | 2.40 | 0.42 |
| 5:CG:169:VAL:HG13 | 5:CG:174:GLN:OE1 | 2.20 | 0.42 |
| 5:CF:317:LEU:HD13 | 5:CG:312:ARG:HH12 | 1.84 | 0.42 |
| 5:CG:389:ASP:N | 5:CG:389:ASP:OD1 | 2.52 | 0.42 |
| 5:CG:430:TRP:HA | 5:CG:431:PRO:C | 2.40 | 0.42 |
| 5:CG:54:ALA:HB2 | 5:CG:71:ASN:O | 2.20 | 0.42 |
| 5:CH:180:VAL:HG22 | 5:CH:181:PHE:H | 1.84 | 0.42 |
| 6:CJ:217:ARG:HE | 6:CJ:219:ALA:C | 2.23 | 0.42 |
| 7:DB:39:ILE:HG22 | 7:DD:44:VAL:HG22 | 2.01 | 0.42 |
| 7:DC:77:THR:OG1 | 7:DC:78:PRO:HD2 | 2.19 | 0.42 |
| 7:DB:188:GLN:NE2 | 7:DD:192:GLN:OE1 | 2.53 | 0.42 |
| 8:DF:134:PRO:HA | 8:DF:157:LEU:HD23 | 2.01 | 0.42 |
| 12:DJ:8:ASN:HA | 12:DJ:12:ILE:HG22 | 2.00 | 0.42 |
| 1:EA:175:THR:O | 1:EA:270:ILE:HG22 | 2.20 | 0.42 |
| 1:EA:347:THR:O | 1:EA:350:SER:N | 2.52 | 0.42 |
| 1:EA:361:GLN:HE21 | 1:EA:456:ASN:HB2 | 1.84 | 0.42 |
| 1:EB:485:VAL:HG11 | 1:EB:650:TYR:CE1 | 2.53 | 0.42 |
| 1:EB:508:ARG:HE | 1:EB:544:ASP:HB2 | 1.83 | 0.42 |
| 2:EC:314:THR:HG23 | 2:EC:317:TYR:HB2 | 2.01 | 0.42 |
| 3:ED:254:ASP:HB3 | 3:ED:257:TYR:CD2 | 2.55 | 0.42 |
| 4:EG:17:ASN:OD1 | 4:EG:18:ALA:N | 2.53 | 0.42 |
| 5:EI:64:TRP:CZ2 | 5:EI:82:PRO:HB2 | 2.54 | 0.42 |
| 5:EJ:117:ILE:HG13 | 5:EJ:118:LYS:H | 1.85 | 0.42 |
| 5:EJ:275:SER:OG | 5:EJ:281:TYR:HA | 2.19 | 0.42 |
| 5:EJ:359:GLU:H | 5:EJ:370:HIS:C | 2.16 | 0.42 |
| 5:EJ:290:SER:CA | 5:EJ:371:PHE:H | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EJ:478:TRP:CH2 | 5:EJ:600:ARG:HB2 | 2.54 | 0.42 |
| 5:EJ:483:GLN:O | 5:EJ:485:LYS:HG2 | 2.19 | 0.42 |
| 4:F:100:ARG:NH2 | 4:F:128:ASP:OD1 | 2.53 | 0.42 |
| 4:F:224:ASP:OD2 | 4:F:227:ASN:HB2 | 2.19 | 0.42 |
| 5:FA:186:TYR:O | 5:FA:227:GLY:HA3 | 2.20 | 0.42 |
| 5:FA:320:LEU:HG | 5:FA:357:SER:CB | 2.49 | 0.42 |
| 5:FA:290:SER:HB3 | 5:FA:370:HIS:HA | 2.01 | 0.42 |
| 6:FB:74:LYS:HG3 | 6:FD:70:ILE:HD11 | 2.02 | 0.42 |
| 6:FB:6:ASN:HB3 | 6:FC:12:SER:HB3 | 2.01 | 0.42 |
| 6:FB:19:GLY:H | 6:FC:13:ARG:CZ | 2.32 | 0.42 |
| 6:FD:217:ARG:HE | 6:FD:219:ALA:C | 2.23 | 0.42 |
| 7:FE:424:ARG:O | 7:FF:504:ARG:NH2 | 2.52 | 0.42 |
| 7:FE:464:ARG:NH2 | 7:FF:492:PRO:HD2 | 2.34 | 0.42 |
| 7:FE:227:VAL:HG23 | 7:FF:225:LYS:HD3 | 2.02 | 0.42 |
| 7:FG:20:PRO:CD | 7:FG:29:ILE:HG21 | 2.49 | 0.42 |
| 7:FF:320:ARG:HG2 | 7:FG:325:TYR:HB2 | 2.01 | 0.42 |
| 7:FF:516:ASN:OD1 | 7:FG:438:GLN:HB2 | 2.19 | 0.42 |
| 7:FG:445:HIS:CD2 | 7:FG:447:HIS:CE1 | 3.06 | 0.42 |
| 1:GD:491:PHE:CE2 | 1:GD:619:GLN:HA | 2.55 | 0.42 |
| 1:GE:508:ARG:HE | 1:GE:544:ASP:HB2 | 1.83 | 0.42 |
| 1:GE:619:GLN:H | 1:GE:619:GLN:CD | 2.21 | 0.42 |
| 2:GF:1005:ARG:HG2 | 2:GF:1006:ASP:O | 2.19 | 0.42 |
| 2:GF:664:PHE:HB2 | 9:IC:15:MET:CB | 2.43 | 0.42 |
| 4:GJ:61:ILE:O | 4:HA:4:GLN:NE2 | 2.48 | 0.42 |
| 4:H:43:GLY:HA2 | 4:H:62:HIS:CE1 | 2.55 | 0.42 |
| 4:HA:190:PRO:HA | 4:HA:262:THR:HA | 2.01 | 0.42 |
| 4:HA:224:ASP:OD2 | 4:HA:227:ASN:HB2 | 2.19 | 0.42 |
| 5:HB:326:MET:HG3 | 5:HB:327:PRO:CD | 2.43 | 0.42 |
| 7:O:233:GLN:HG3 | 5:HB:347:GLY:HA2 | 2.02 | 0.42 |
| 5:HB:261:ARG:HB2 | 5:HB:383:ILE:HB | 2.01 | 0.42 |
| 5:HB:89:TYR:HB3 | 5:HC:98:VAL:HG13 | 2.02 | 0.42 |
| 5:HC:117:ILE:HG13 | 5:HC:118:LYS:H | 1.85 | 0.42 |
| 5:HC:430:TRP:HA | 5:HC:431:PRO:C | 2.40 | 0.42 |
| 5:HD:186:TYR:HB3 | 5:HD:227:GLY:C | 2.40 | 0.42 |
| 5:HD:169:VAL:O | 5:HD:238:ILE:HA | 2.19 | 0.42 |
| 5:HD:320:LEU:HG | 5:HD:357:SER:CB | 2.49 | 0.42 |
| 5:HB:318:GLN:NE2 | 6:HG:4:LEU:O | 2.50 | 0.42 |
| 7:HH:111:ASN:ND2 | 7:HH:114:SER:HB3 | 2.34 | 0.42 |
| 7:HH:190:VAL:HB | 7:HI:188:GLN:C | 2.40 | 0.42 |
| 7:HH:192:GLN:HG3 | 7:HI:188:GLN:CD | 2.40 | 0.42 |
| 7:HI:32:VAL:O | 7:HI:36:ILE:N | 2.42 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HI:451:PHE:HD1 | 7:HI:469:VAL:HG13 | 1.85 | 0.42 |
| 7:HI:515:TRP:CE3 | 7:HJ:439:ILE:HA | 2.55 | 0.42 |
| 7:HJ:58:LEU:HD21 | 7:HJ:75:ALA:H | 1.84 | 0.42 |
| 5:I:193:VAL:O | 5:I:199:GLU:N | 2.46 | 0.42 |
| 8:IA:25:ILE:O | 8:IA:26:SER:HB3 | 2.20 | 0.42 |
| 11:IE:71:TRP:O | 11:IE:74:LEU:N | 2.53 | 0.42 |
| 12:IF:15:ASP:O | 12:IF:16:PHE:CD1 | 2.73 | 0.42 |
| 5:J:290:SER:CA | 5:J:371:PHE:H | 2.33 | 0.42 |
| 5:J:460:TYR:CE1 | 5:K:458:THR:HG23 | 2.55 | 0.42 |
| 5:J:483:GLN:O | 5:J:485:LYS:HG2 | 2.19 | 0.42 |
| 5:K:181:PHE:HE2 | 5:K:246:THR:HG22 | 1.85 | 0.42 |
| 5:K:288:MET:CE | 5:K:292:PRO:HD3 | 2.50 | 0.42 |
| 5:K:497:PRO:HG2 | 5:K:498:ASN:ND2 | 2.35 | 0.42 |
| 6:L:217:ARG:HE | 6:L:219:ALA:C | 2.23 | 0.42 |
| 6:M:135:GLU:O | 6:M:139:SER:N | 2.26 | 0.42 |
| 6:M:82:VAL:HG23 | 6:M:187:LYS:HE3 | 2.01 | 0.42 |
| 7:O:176:ILE:HG23 | 7:O:177:ALA:H | 1.84 | 0.42 |
| 7:O:32:VAL:HG22 | 7:O:36:ILE:HG12 | 2.01 | 0.42 |
| 7:O:363:HIS:CD2 | 7:O:396:ARG:HD3 | 2.54 | 0.42 |
| 7:O:453:GLU:CD | 7:O:471:THR:H | 2.18 | 0.42 |
| 7:O:75:ALA:HB1 | 7:P:75:ALA:HB1 | 2.01 | 0.42 |
| 7:P:31:ASP:CG | 7:P:34:ALA:H | 2.18 | 0.42 |
| 7:P:77:THR:HG21 | 7:Q:72:ASN:CG | 2.40 | 0.42 |
| 5:J:196:ARG:HH22 | 7:Q:9:VAL:HG12 | 1.81 | 0.42 |
| 10:U:322:ASP:O | 10:U:342:PHE:HB2 | 2.19 | 0.42 |
| 12:W:182:GLN:N | 12:W:182:GLN:OE1 | 4.91 | 0.42 |
| 1:Y:322:ILE:HG13 | 1:Y:323:GLU:N | 2.35 | 0.42 |
| 1:Y:533:ASP:O | 1:Y:535:LEU:N | 2.53 | 0.42 |
| 13:YA:330[E]:ILE:HD12 | 13:YA:336[E]:LEU:HD12 | 2.01 | 0.42 |
| 13:YA:38[C]:GLN:O | 13:YA:46[C]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:132[A]:LEU:O | 13:YA:390[A]:VAL:HG11 | 2.19 | 0.42 |
| 13:YA:132[F]:LEU:O | 13:YA:390[F]:VAL:HG11 | 2.19 | 0.42 |
| 13:YA:569[C]:GLY:HA2 | 13:YB:561[C]:SER:O | 2.18 | 0.42 |
| 13:YB:195[D]:GLU:HG2 | 13:YB:197[D]:TYR:CE2 | 2.54 | 0.42 |
| 13:YB:252[F]:MET:HB3 | 13:YB:252[F]:MET:HE3 | 1.74 | 0.42 |
| 13:YB:280[A]:MET:O | 13:YB:284[A]:MET:HG2 | 2.19 | 0.42 |
| 13:YB:280[F]:MET:O | 13:YB:284[F]:MET:HG2 | 2.20 | 0.42 |
| 13:YB:320[C]:THR:HG22 | 13:YB:323[C]:ARG:HB3 | 2.00 | 0.42 |
| 13:YB:321[B]:LYS:HD3 | 13:YC:452[B]:GLY:CA | 2.47 | 0.42 |
| 13:YB:320[F]:THR:HG22 | 13:YB:323[F]:ARG:HB3 | 2.00 | 0.42 |
| 13:YB:330[B]:ILE:HD12 | 13:YB:336[B]:LEU:HD12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:34[D]:LEU:HD13 | 14:YE:163[D]:THR:CG2 | 2.47 | 0.42 |
| 13:YB:132[C]:LEU:O | 13:YB:390[C]:VAL:HG11 | 2.19 | 0.42 |
| 13:YB:389[E]:TYR:O | 13:YB:405[E]:ASP:HB2 | 2.19 | 0.42 |
| 13:YB:476[A]:GLY:HA3 | 13:YC:469[A]:ASN:HA | 2.00 | 0.42 |
| 13:YB:515[D]:LYS:HG3 | 13:YC:507[D]:GLU:HA | 2.02 | 0.42 |
| 13:YA:551[A]:THR:O | 13:YB:543[A]:ASP:HA | 2.19 | 0.42 |
| 13:YB:546[A]:VAL:HG11 | 13:YC:542[A]:VAL:HG13 | 2.01 | 0.42 |
| 13:YB:564[F]:GLN:HG3 | 13:YB:566[F]:THR:HG22 | 2.01 | 0.42 |
| 13:YB:564[E]:GLN:HG3 | 13:YB:566[E]:THR:HG22 | 2.01 | 0.42 |
| 13:YB:76[E]:PRO:HB3 | 13:YB:98[E]:GLY:C | 2.40 | 0.42 |
| 13:YC:132[B]:LEU:O | 13:YC:390[B]:VAL:HG11 | 2.19 | 0.42 |
| 13:YC:147[B]:ILE:HD11 | 13:YC:188[B]:LEU:HG | 2.00 | 0.42 |
| 13:YC:296[E]:LEU:HA | 13:YC:296[E]:LEU:HD12 | 1.84 | 0.42 |
| 13:YC:330[D]:ILE:HD12 | 13:YC:336[D]:LEU:HD12 | 2.01 | 0.42 |
| 13:YC:439[B]:TYR:HB3 | 13:YC:441[B]:ILE:CD1 | 2.50 | 0.42 |
| 13:YC:454[B]:LYS:C | 13:YC:455[B]:LYS:HG3 | 2.39 | 0.42 |
| 13:YB:454[A]:LYS:NZ | 13:YC:464[A]:TYR:OH | 2.53 | 0.42 |
| 13:YB:454[F]:LYS:NZ | 13:YC:464[F]:TYR:OH | 2.52 | 0.42 |
| 13:YC:47[B]:ILE:HG23 | 14:YF:123[B]:PRO:CG | 2.47 | 0.42 |
| 13:YA:550[D]:TRP:HB2 | 13:YC:554[D]:MET:HG3 | 2.02 | 0.42 |
| 13:YC:76[E]:PRO:HB3 | 13:YC:98[E]:GLY:C | 2.40 | 0.42 |
| 13:YC:83[A]:TYR:OH | 13:YC:85[A]:HIS:HE1 | 2.03 | 0.42 |
| 14:YD:114[A]:SER:HA | 14:YD:167[A]:GLU:OE1 | 2.20 | 0.42 |
| 14:YD:114[E]:SER:HA | 14:YD:167[E]:GLU:OE1 | 2.19 | 0.42 |
| 14:YD:112[C]:ILE:HB | 14:YD:140[C]:TYR:OH | 2.20 | 0.42 |
| 14:YD:86[C]:ARG:HD2 | 14:YD:192[C]:ILE:HD12 | 2.01 | 0.42 |
| 11:BF:175:SER:HA | 14:YD:217[C]:SER:HB2 | 2.01 | 0.42 |
| 14:YD:234[A]:PHE:HD1 | 14:YE:97[A]:VAL:HG12 | 1.84 | 0.42 |
| 14:YD:360[D]:ASN:HD22 | 14:YD:360[D]:ASN:N | 1.97 | 0.42 |
| 14:YE:124[C]:PHE:CZ | 14:YE:135[C]:MET:HG2 | 2.55 | 0.42 |
| 14:YE:112[A]:ILE:HB | 14:YE:140[A]:TYR:OH | 2.20 | 0.42 |
| 13:YB:26[E]:ARG:HD3 | 14:YE:259[E]:LEU:HD21 | 2.01 | 0.42 |
| 14:YE:290[E]:ASN:OD1 | 14:YE:290[E]:ASN:C | 2.58 | 0.42 |
| 14:YF:114[B]:SER:HA | 14:YF:167[B]:GLU:OE1 | 2.20 | 0.42 |
| 14:YF:172[D]:TYR:CZ | 14:YF:176[D]:VAL:HG21 | 2.54 | 0.42 |
| 14:YF:43[A]:SER:O | 14:YF:189[A]:TRP:HB2 | 2.20 | 0.42 |
| 14:YF:75[A]:ALA:HB2 | 14:YF:83[A]:VAL:HA | 2.00 | 0.42 |
| 14:YF:86[E]:ARG:HD2 | 14:YF:192[E]:ILE:HD12 | 2.01 | 0.42 |
| 2:Z:321:VAL:HA | 2:Z:326:VAL:HA | 2.01 | 0.42 |
| 2:Z:416:VAL:HG23 | 2:Z:417:PHE:H | 1.84 | 0.42 |
| 2:Z:784:GLN:HG2 | 2:Z:830:ARG:CB | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:872:SER:HA | 2:Z:875:TRP:CD1 | 2.55 | 0.42 |
| 2:Z:906:LEU:HD12 | 2:Z:907:LYS:N | 2.35 | 0.42 |
| 2:Z:967:ASP:N | 2:Z:967:ASP:OD1 | 2.53 | 0.42 |
| 1:A:390:GLU:O | 1:A:394:ASN:ND2 | 2.53 | 0.42 |
| 4:AA:25:PHE:HB2 | 4:AB:15:ILE:HD13 | 2.02 | 0.42 |
| 5:AD:104:VAL:HG13 | 5:AD:105:ASN:H | 1.84 | 0.42 |
| 5:AD:138:CYS:SG | 5:AD:140:PRO:HD2 | 2.59 | 0.42 |
| 5:AD:480:LEU:HD23 | 5:AD:480:LEU:HA | 1.81 | 0.42 |
| 5:AD:49:TRP:HH2 | 5:AD:96:ARG:HE | 1.67 | 0.42 |
| 5:AE:207:SER:O | 5:AE:210:SER:OG | 2.33 | 0.42 |
| 6:AG:43:LEU:O | 6:AH:111:GLY:HA3 | 2.19 | 0.42 |
| 7:AI:183:ALA:O | 7:AI:187:ASP:HB2 | 2.19 | 0.42 |
| 7:AI:192:GLN:HG3 | 7:AJ:188:GLN:CD | 2.40 | 0.42 |
| 7:AI:503:ASN:ND2 | 7:BA:445:HIS:HB2 | 2.35 | 0.42 |
| 7:AI:143:LYS:HG2 | 7:AJ:138:SER:C | 2.40 | 0.42 |
| 7:AJ:255:SER:HB2 | 7:AJ:261:GLY:O | 2.20 | 0.42 |
| 7:AI:300:LEU:HB3 | 7:AJ:302:ILE:HD13 | 2.01 | 0.42 |
| 7:AJ:347:MET:HE3 | 7:AJ:347:MET:HB2 | 1.77 | 0.42 |
| 1:B:174:ARG:HA | 1:B:270:ILE:O | 2.19 | 0.42 |
| 1:B:341:THR:OG1 | 1:B:342:ALA:N | 2.51 | 0.42 |
| 1:B:429:LEU:O | 1:B:429:LEU:HD12 | 2.19 | 0.42 |
| 7:BA:218:SER:O | 7:BA:227:VAL:HG22 | 2.19 | 0.42 |
| 8:BC:91:ILE:HG22 | 8:BC:107:TYR:HB3 | 2.01 | 0.42 |
| 9:BD:20:ASN:C | 9:BD:20:ASN:OD1 | 2.57 | 0.42 |
| 9:BD:64:ASN:O | 9:BD:69:THR:HG21 | 2.19 | 0.42 |
| 11:BF:133:TRP:CE2 | 11:BF:150:LEU:HD11 | 2.55 | 0.42 |
| 11:BF:177:ILE:HG23 | 11:BF:178:ASN:N | 2.35 | 0.42 |
| 1:BH:315:GLY:HA2 | 1:BH:356:ILE:CD1 | 2.50 | 0.42 |
| 1:BH:390:GLU:O | 1:BH:394:ASN:ND2 | 2.53 | 0.42 |
| 1:BI:189:ASP:O | 1:BI:192:ILE:HG23 | 2.20 | 0.42 |
| 2:BJ:618:PHE:CD1 | 2:BJ:619:LEU:HB2 | 2.55 | 0.42 |
| 1:BI:403:PRO:HB2 | 2:BJ:888:PHE:CD2 | 2.54 | 0.42 |
| 2:C:145:ALA:HB2 | 2:C:542:THR:CB | 2.48 | 0.42 |
| 2:C:784:GLN:HG2 | 2:C:830:ARG:CB | 2.50 | 0.42 |
| 3:CA:254:ASP:HB3 | 3:CA:257:TYR:CD2 | 2.55 | 0.42 |
| 3:CB:235:ASP:O | 3:CB:236:PHE:HB2 | 2.20 | 0.42 |
| 4:CD:43:GLY:HA2 | 4:CD:62:HIS:CE1 | 2.55 | 0.42 |
| 3:CA:201:ASN:OD1 | 5:CF:10:VAL:HG21 | 2.20 | 0.42 |
| 5:CF:322:GLY:HA2 | 5:CF:360:THR:N | 2.34 | 0.42 |
| 5:CG:117:ILE:HG13 | 5:CG:118:LYS:H | 1.85 | 0.42 |
| 5:CG:48:ALA:C | 5:CG:49:TRP:CD1 | 2.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:137:TYR:HA | 5:CH:143:TRP:HD1 | 1.82 | 0.42 |
| 5:CG:255:ARG:HH21 | 5:CH:249:ASP:HB2 | 1.85 | 0.42 |
| 5:CH:394:LEU:HA | 5:CH:394:LEU:HD23 | 1.91 | 0.42 |
| 6:CI:141:THR:HG22 | 6:DA:43:LEU:HD11 | 2.01 | 0.42 |
| 6:CI:6:ASN:HB3 | 6:CJ:12:SER:CB | 2.50 | 0.42 |
| 7:DB:260:ARG:HD3 | 7:DD:262:VAL:HG23 | 2.02 | 0.42 |
| 7:DD:111:ASN:ND2 | 7:DD:114:SER:HB3 | 2.34 | 0.42 |
| 7:DD:77:THR:OG1 | 7:DD:78:PRO:HD2 | 2.20 | 0.42 |
| 8:DF:89:GLN:HB3 | 8:DF:134:PRO:CG | 2.50 | 0.42 |
| 12:DJ:15:ASP:O | 12:DJ:16:PHE:CD1 | 2.73 | 0.42 |
| 1:EA:209:TRP:HD1 | 1:EA:225:TYR:CE1 | 2.35 | 0.42 |
| 1:EA:306:ASP:OD1 | 1:EA:306:ASP:N | 2.52 | 0.42 |
| 1:EA:390:GLU:O | 1:EA:394:ASN:ND2 | 2.53 | 0.42 |
| 1:EB:148:ARG:HG2 | 1:EB:149:GLU:HG3 | 2.01 | 0.42 |
| 1:EB:158:ASN:CG | 1:EB:160:GLN:HG2 | 2.40 | 0.42 |
| 1:EB:189:ASP:O | 1:EB:192:ILE:HG23 | 2.20 | 0.42 |
| 1:EB:219:SER:O | 1:EB:220:THR:OG1 | 2.29 | 0.42 |
| 2:EC:251:ASP:OD2 | 2:EC:252:LYS:HG3 | 2.20 | 0.42 |
| 3:ED:292:ALA:HB1 | 3:ED:297:TYR:CZ | 2.54 | 0.42 |
| 4:EF:100:ARG:NH2 | 4:EF:128:ASP:OD1 | 2.53 | 0.42 |
| 4:EG:209:VAL:HG13 | 4:EG:271:GLY:O | 2.19 | 0.42 |
| 5:EJ:116:THR:HG22 | 5:EJ:121:ALA:HB2 | 2.02 | 0.42 |
| 5:EJ:138:CYS:SG | 5:EJ:140:PRO:HD2 | 2.60 | 0.42 |
| 5:EJ:154:ILE:HD12 | 5:EJ:155:THR:N | 2.35 | 0.42 |
| 5:EJ:48:ALA:C | 5:EJ:49:TRP:CD1 | 2.93 | 0.42 |
| 4:F:251:ASN:N | 4:F:266:SER:O | 2.53 | 0.42 |
| 4:F:44:ASP:O | 4:F:59:GLN:NE2 | 2.52 | 0.42 |
| 7:FE:111:ASN:ND2 | 7:FE:114:SER:HB3 | 2.34 | 0.42 |
| 7:FE:497:ASN:OD1 | 7:FE:500:TYR:N | 2.53 | 0.42 |
| 7:FE:162:PRO:CB | 7:FF:150:ALA:HA | 2.48 | 0.42 |
| 7:FF:255:SER:HB2 | 7:FF:261:GLY:O | 2.20 | 0.42 |
| 7:FG:166:GLN:O | 7:FG:170:ILE:HB | 2.20 | 0.42 |
| 7:FE:346:ILE:O | 7:FG:348:MET:HB2 | 2.20 | 0.42 |
| 7:FG:4:ASN:O | 7:FG:8:HIS:N | 2.48 | 0.42 |
| 7:FG:58:LEU:HD21 | 7:FG:75:ALA:H | 1.84 | 0.42 |
| 7:FF:77:THR:HA | 7:FG:74:LYS:O | 2.20 | 0.42 |
| 9:FJ:20:ASN:C | 9:FJ:20:ASN:OD1 | 2.57 | 0.42 |
| 9:FJ:64:ASN:O | 9:FJ:69:THR:HG21 | 2.19 | 0.42 |
| 4:G:61:ILE:O | 4:H:4:GLN:NE2 | 2.50 | 0.42 |
| 11:GB:43:TYR:O | 11:GB:44:ARG:HB2 | 2.19 | 0.42 |
| 1:GD:192:ILE:HG22 | 1:GD:272:TYR:CE1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:347:THR:O | 1:GD:350:SER:N | 2.52 | 0.42 |
| 2:GF:439:LYS:HG3 | 2:GF:440:LEU:HD12 | 2.01 | 0.42 |
| 2:GF:480:LEU:CD2 | 2:GF:488:MET:HB2 | 2.49 | 0.42 |
| 2:GF:821:ILE:O | 2:GF:824:GLN:NE2 | 2.32 | 0.42 |
| 2:GF:872:SER:HA | 2:GF:875:TRP:CD1 | 2.55 | 0.42 |
| 3:GG:194:ILE:HG12 | 3:GG:223:TRP:HZ3 | 1.84 | 0.42 |
| 4:GI:192:PHE:O | 4:GI:261:VAL:N | 2.51 | 0.42 |
| 4:GI:43:GLY:HA2 | 4:GI:62:HIS:CE1 | 2.55 | 0.42 |
| 4:HA:17:ASN:OD1 | 4:HA:18:ALA:N | 2.53 | 0.42 |
| 4:HA:251:ASN:N | 4:HA:266:SER:O | 2.53 | 0.42 |
| 5:HB:450:PHE:CZ | 5:HB:454:TYR:HD2 | 2.38 | 0.42 |
| 5:HC:102:TRP:CD1 | 5:HC:102:TRP:N | 2.86 | 0.42 |
| 5:HC:215:PRO:HB3 | 5:HC:229:ASN:C | 2.39 | 0.42 |
| 5:HC:34:TYR:OH | 5:HC:41:ASP:C | 2.58 | 0.42 |
| 5:HC:400:ILE:HG12 | 5:HD:402:GLU:OE2 | 2.19 | 0.42 |
| 6:HE:64:ILE:HG23 | 6:HE:217:ARG:HH12 | 1.84 | 0.42 |
| 7:HH:183:ALA:O | 7:HH:187:ASP:HB2 | 2.19 | 0.42 |
| 7:HI:227:VAL:CG2 | 7:HJ:225:LYS:HB3 | 2.49 | 0.42 |
| 7:HI:491:ASP:HB2 | 7:HI:496:ARG:HG2 | 2.01 | 0.42 |
| 7:HI:516:ASN:OD1 | 7:HJ:438:GLN:HB2 | 2.20 | 0.42 |
| 5:I:304:ILE:HG12 | 5:I:305:ASN:O | 2.20 | 0.42 |
| 5:I:331:CYS:HA | 5:I:349:TRP:CZ2 | 2.46 | 0.42 |
| 5:I:89:TYR:HB3 | 5:J:98:VAL:HG13 | 2.02 | 0.42 |
| 9:IC:58:SER:O | 9:IC:62:PHE:N | 2.34 | 0.42 |
| 9:IC:72:THR:OG1 | 10:ID:126:ASN:ND2 | 2.45 | 0.42 |
| 11:IE:43:TYR:CE2 | 11:IE:180:PHE:HB2 | 2.49 | 0.42 |
| 12:IF:117:ALA:O | 12:IF:120:SER:OG | 2.24 | 0.42 |
| 5:J:102:TRP:N | 5:J:102:TRP:CD1 | 2.86 | 0.42 |
| 5:J:116:THR:HG22 | 5:J:121:ALA:HB2 | 2.02 | 0.42 |
| 5:J:250:GLY:N | 5:K:158:ASP:HB3 | 2.35 | 0.42 |
| 5:J:478:TRP:CH2 | 5:J:600:ARG:HB2 | 2.54 | 0.42 |
| 5:K:150:GLN:HG3 | 5:K:152:ASP:HB3 | 2.01 | 0.42 |
| 5:K:186:TYR:HB3 | 5:K:227:GLY:CA | 2.49 | 0.42 |
| 5:K:186:TYR:O | 5:K:227:GLY:HA3 | 2.20 | 0.42 |
| 5:K:192:ARG:HB2 | 5:K:245:GLU:H | 1.84 | 0.42 |
| 5:J:326:MET:HE1 | 5:K:264:ARG:HB3 | 2.01 | 0.42 |
| 5:K:258:TYR:HD1 | 5:K:386:PHE:HD1 | 1.66 | 0.42 |
| 5:K:542:LEU:HA | 5:K:542:LEU:HD23 | 1.88 | 0.42 |
| 6:L:87:TYR:N | 6:L:181:GLU:O | 2.32 | 0.42 |
| 6:L:6:ASN:HB3 | 6:M:12:SER:HB3 | 2.02 | 0.42 |
| 7:O:255:SER:N | 7:O:278:SER:OG | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:190:VAL:HB | 7:P:188:GLN:C | 2.40 | 0.42 |
| 7:Q:240:ASN:HB3 | 7:Q:243:VAL:HG22 | 2.00 | 0.42 |
| 7:Q:493:GLU:HG3 | 7:Q:496:ARG:HH21 | 1.84 | 0.42 |
| 7:O:429:CYS:HA | 7:Q:511:GLU:OE1 | 2.19 | 0.42 |
| 1:X:306:ASP:OD1 | 1:X:306:ASP:N | 2.52 | 0.42 |
| 1:Y:530:LEU:HD12 | 1:Y:532:GLU:H | 1.84 | 0.42 |
| 13:YA:293[D]:ASN:HA | 13:YA:296[D]:LEU:HB2 | 2.01 | 0.42 |
| 13:YA:439[C]:TYR:HB3 | 13:YA:441[C]:ILE:CD1 | 2.49 | 0.42 |
| 13:YA:454[F]:LYS:C | 13:YA:455[F]:LYS:HG3 | 2.40 | 0.42 |
| 13:YA:551[B]:THR:O | 13:YB:543[B]:ASP:HA | 2.19 | 0.42 |
| 13:YA:564[B]:GLN:HG3 | 13:YA:566[B]:THR:HG22 | 2.01 | 0.42 |
| 13:YB:127[A]:ASN:ND2 | 13:YB:129[A]:THR:OG1 | 2.53 | 0.42 |
| 13:YB:280[E]:MET:O | 13:YB:284[E]:MET:HG2 | 2.19 | 0.42 |
| 13:YB:293[D]:ASN:HA | 13:YB:296[D]:LEU:HB2 | 2.01 | 0.42 |
| 13:YB:320[B]:THR:HG22 | 13:YB:323[B]:ARG:HB3 | 2.00 | 0.42 |
| 13:YB:410[C]:GLU:O | 13:YB:426[C]:PRO:HA | 2.20 | 0.42 |
| 13:YB:439[D]:TYR:HB3 | 13:YB:441[D]:ILE:CD1 | 2.50 | 0.42 |
| 13:YB:442[D]:THR:HB | 13:YC:434[D]:THR:HB | 2.01 | 0.42 |
| 13:YB:534[F]:LEU:HD11 | 13:YB:536[F]:TRP:NE1 | 2.32 | 0.42 |
| 13:YB:564[A]:GLN:HG3 | 13:YB:566[A]:THR:HG22 | 2.01 | 0.42 |
| 13:YB:83[F]:TYR:OH | 13:YB:85[F]:HIS:HE1 | 2.02 | 0.42 |
| 13:YC:180[A]:LEU:HA | 13:YC:180[A]:LEU:HD13 | 1.76 | 0.42 |
| 13:YC:293[A]:ASN:HA | 13:YC:296[A]:LEU:HB2 | 2.01 | 0.42 |
| 13:YC:132[A]:LEU:O | 13:YC:390[A]:VAL:HG11 | 2.19 | 0.42 |
| 13:YA:445[E]:ASP:HA | 13:YC:453[E]:ASP:O | 2.20 | 0.42 |
| 13:YC:38[E]:GLN:O | 13:YC:46[E]:GLY:HA2 | 2.20 | 0.42 |
| 13:YB:515[B]:LYS:HG3 | 13:YC:507[B]:GLU:HA | 2.02 | 0.42 |
| 13:YC:564[D]:GLN:HG3 | 13:YC:566[D]:THR:HG22 | 2.01 | 0.42 |
| 13:YC:564[C]:GLN:HG3 | 13:YC:566[C]:THR:HG22 | 2.01 | 0.42 |
| 13:YC:81[D]:ARG:HD3 | 14:YE:261[D]:SER:HA | 2.02 | 0.42 |
| 14:YD:172[F]:TYR:CZ | 14:YD:176[F]:VAL:HG21 | 2.54 | 0.42 |
| 14:YD:17[B]:PHE:HE2 | 14:YD:26[B]:ASN:HA | 1.85 | 0.42 |
| 14:YD:290[C]:ASN:C | 14:YD:290[C]:ASN:OD1 | 2.58 | 0.42 |
| 14:YD:38[E]:LEU:HD12 | 14:YD:38[E]:LEU:HA | 1.63 | 0.42 |
| 14:YE:112[C]:ILE:HB | 14:YE:140[C]:TYR:OH | 2.20 | 0.42 |
| 14:YE:124[D]:PHE:CZ | 14:YE:135[D]:MET:HG2 | 2.55 | 0.42 |
| 14:YE:43[C]:SER:O | 14:YE:189[C]:TRP:HB2 | 2.20 | 0.42 |
| 14:YE:210[F]:PRO:HB2 | 14:YE:228[F]:TYR:CD2 | 2.55 | 0.42 |
| 14:YE:75[D]:ALA:HB2 | 14:YE:83[D]:VAL:HA | 2.01 | 0.42 |
| 14:YF:114[C]:SER:HA | 14:YF:167[C]:GLU:OE1 | 2.20 | 0.42 |
| 14:YF:114[E]:SER:HA | 14:YF:167[E]:GLU:OE1 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:112[A]:ILE:HB | 14:YF:140[A]:TYR:OH | 2.20 | 0.42 |
| 14:YF:259[B]:LEU:HD23 | 14:YF:259[B]:LEU:HA | 1.82 | 0.42 |
| 2:Z:146:LEU:HD12 | 2:Z:146:LEU:C | 2.39 | 0.42 |
| 1:A:192:ILE:HG22 | 1:A:272:TYR:CE1 | 2.54 | 0.42 |
| 4:AA:201:LYS:NZ | 4:AA:220:ASN:OD1 | 2.37 | 0.42 |
| 4:AA:209:VAL:HG13 | 4:AA:271:GLY:O | 2.19 | 0.42 |
| 5:AC:472:TYR:O | 5:AD:416:ILE:HD12 | 2.20 | 0.42 |
| 5:AE:117:ILE:HG13 | 5:AE:118:LYS:H | 1.84 | 0.42 |
| 5:AD:250:GLY:N | 5:AE:158:ASP:HB3 | 2.35 | 0.42 |
| 5:AE:215:PRO:HB3 | 5:AE:229:ASN:O | 2.19 | 0.42 |
| 5:AE:71:ASN:ND2 | 5:AE:73:SER:OG | 2.52 | 0.42 |
| 5:AD:340:VAL:HG22 | 6:AH:172:SER:O | 2.20 | 0.42 |
| 6:AH:88:TRP:HB3 | 6:AH:90:PHE:CE1 | 2.55 | 0.42 |
| 7:AI:248:ALA:O | 7:AI:252:GLY:N | 2.44 | 0.42 |
| 7:AI:503:ASN:ND2 | 7:BA:446:LYS:H | 2.18 | 0.42 |
| 7:AI:65:GLU:O | 7:AI:69:GLY:N | 2.48 | 0.42 |
| 7:AJ:480:ARG:HD3 | 7:BA:462:ASN:ND2 | 2.34 | 0.42 |
| 7:AJ:491:ASP:HB2 | 7:AJ:496:ARG:HG2 | 2.01 | 0.42 |
| 7:AI:425:LEU:HD11 | 7:AJ:505:PRO:O | 2.19 | 0.42 |
| 1:B:348:PHE:HZ | 1:B:399:TYR:HD2 | 1.65 | 0.42 |
| 1:B:403:PRO:HB2 | 2:C:888:PHE:CD2 | 2.55 | 0.42 |
| 7:AI:185:GLU:HA | 7:BA:193:LEU:HB2 | 2.01 | 0.42 |
| 7:BA:196:VAL:HG22 | 7:BA:214:THR:HG22 | 2.02 | 0.42 |
| 8:BB:18:PRO:HD3 | 8:DE:151:GLN:N | 2.34 | 0.42 |
| 8:BC:134:PRO:HA | 8:BC:157:LEU:HD23 | 2.01 | 0.42 |
| 11:BF:6:PHE:HE1 | 11:BF:188:MET:O | 2.03 | 0.42 |
| 1:BH:222:THR:C | 1:BH:223:ILE:HG12 | 2.40 | 0.42 |
| 1:BH:472:ASP:O | 1:BH:473:HIS:CG | 2.73 | 0.42 |
| 1:BH:592:ILE:O | 1:BH:608:LYS:HD2 | 2.19 | 0.42 |
| 1:BI:299:ASN:OD1 | 1:BI:300:ILE:N | 2.52 | 0.42 |
| 2:BJ:312:THR:OG1 | 2:BJ:368:MET:SD | 2.73 | 0.42 |
| 2:BJ:976:SER:C | 2:BJ:977:ILE:HG13 | 2.40 | 0.42 |
| 2:C:300:LEU:N | 2:C:301:PRO:HD3 | 2.34 | 0.42 |
| 1:B:56:LEU:HA | 2:C:653:MET:HE1 | 2.02 | 0.42 |
| 2:C:724:ALA:C | 2:C:726:PHE:H | 2.20 | 0.42 |
| 2:C:798:ILE:HG12 | 2:C:811:VAL:HG12 | 2.00 | 0.42 |
| 2:C:872:SER:HA | 2:C:875:TRP:CD1 | 2.55 | 0.42 |
| 2:C:980:GLY:C | 2:C:983:PRO:HD2 | 2.40 | 0.42 |
| 2:BJ:986:ARG:HH12 | 3:CA:323:ASP:HB2 | 1.85 | 0.42 |
| 4:CE:147:THR:HB | 4:CE:163:SER:HG | 1.85 | 0.42 |
| 5:CF:202:TYR:CD1 | 5:CF:225:LEU:HD12 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:195:HIS:NE2 | 5:CF:236:CYS:SG | 2.85 | 0.42 |
| 5:CG:215:PRO:HB3 | 5:CG:229:ASN:C | 2.39 | 0.42 |
| 5:CG:290:SER:CA | 5:CG:371:PHE:H | 2.33 | 0.42 |
| 5:CG:478:TRP:CH2 | 5:CG:600:ARG:HB2 | 2.54 | 0.42 |
| 5:CG:305:ASN:HB3 | 5:CH:255:ARG:HH12 | 1.84 | 0.42 |
| 5:CH:311:VAL:HA | 5:CH:382:ASN:O | 2.20 | 0.42 |
| 7:DB:160:MET:HG3 | 7:DB:164:LYS:HZ1 | 1.83 | 0.42 |
| 7:DB:160:MET:HA | 7:DB:164:LYS:HZ1 | 1.85 | 0.42 |
| 7:DB:464:ARG:NH2 | 7:DC:492:PRO:HD2 | 2.35 | 0.42 |
| 6:AF:77:VAL:CG2 | 7:DC:167:GLN:HE21 | 2.28 | 0.42 |
| 7:DC:20:PRO:HB3 | 7:DC:29:ILE:HG13 | 2.01 | 0.42 |
| 7:DC:515:TRP:CE3 | 7:DD:439:ILE:HA | 2.54 | 0.42 |
| 7:DD:110:VAL:HG12 | 7:DD:111:ASN:H | 1.84 | 0.42 |
| 8:DE:134:PRO:HA | 8:DE:157:LEU:HD23 | 2.01 | 0.42 |
| 1:BH:53:LEU:HB2 | 9:DG:23:VAL:HG23 | 2.02 | 0.42 |
| 11:DI:133:TRP:CE2 | 11:DI:150:LEU:HD11 | 2.55 | 0.42 |
| 12:DJ:171:TYR:HD1 | 12:DJ:239:PHE:CE2 | 2.38 | 0.42 |
| 1:EA:105:ALA:HB2 | 1:EA:275:THR:HG21 | 2.02 | 0.42 |
| 1:EA:315:GLY:HA2 | 1:EA:356:ILE:CD1 | 2.50 | 0.42 |
| 1:EA:491:PHE:CE2 | 1:EA:619:GLN:HA | 2.55 | 0.42 |
| 1:EB:322:ILE:HG13 | 1:EB:323:GLU:N | 2.35 | 0.42 |
| 1:EB:423:THR:O | 1:EB:476:ILE:N | 2.45 | 0.42 |
| 1:EB:448:TYR:HD1 | 1:EB:452:VAL:HG11 | 1.85 | 0.42 |
| 1:EB:496:GLU:HG2 | 1:EB:496:GLU:H | 1.57 | 0.42 |
| 2:EC:380:ILE:HB | 2:EC:396:ILE:HG21 | 2.01 | 0.42 |
| 2:EC:509:TYR:HD2 | 3:GH:229:LEU:HD23 | 1.84 | 0.42 |
| 2:EC:526:ILE:HD12 | 2:EC:526:ILE:HA | 1.84 | 0.42 |
| 2:EC:73:ASP:HB3 | 2:EC:76:THR:HG21 | 2.02 | 0.42 |
| 2:EC:980:GLY:C | 2:EC:983:PRO:HD2 | 2.40 | 0.42 |
| 3:ED:308:GLU:OE1 | 3:EE:15:LYS:NZ | 2.41 | 0.42 |
| 2:BJ:448:PHE:CE2 | 3:ED:66:LEU:HD11 | 2.55 | 0.42 |
| 4:EF:251:ASN:N | 4:EF:266:SER:O | 2.53 | 0.42 |
| 5:EI:133:LEU:HA | 5:EI:133:LEU:HD23 | 1.81 | 0.42 |
| 5:FA:137:TYR:HA | 5:FA:143:TRP:HD1 | 1.82 | 0.42 |
| 5:FA:288:MET:CE | 5:FA:292:PRO:HD3 | 2.50 | 0.42 |
| 5:FA:368:ILE:HG13 | 5:FA:369:LEU:N | 2.35 | 0.42 |
| 5:EI:394:LEU:HD22 | 5:FA:395:THR:HA | 2.02 | 0.42 |
| 5:EI:408:VAL:HG23 | 5:FA:409:SER:O | 2.20 | 0.42 |
| 5:FA:409:SER:OG | 5:FA:411:GLY:N | 2.52 | 0.42 |
| 6:FB:195:LEU:HA | 6:FB:215:PHE:HD1 | 1.85 | 0.42 |
| 7:FE:318:THR:HA | 7:FF:323:GLY:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FG:111:ASN:ND2 | 7:FG:114:SER:HB3 | 2.34 | 0.42 |
| 7:FG:405:ARG:HB2 | 7:FG:430:THR:OG1 | 2.20 | 0.42 |
| 4:F:171:LYS:N | 4:G:164:ILE:O | 2.46 | 0.42 |
| 4:F:54:THR:HA | 4:G:7:LYS:O | 2.20 | 0.42 |
| 1:GD:278:ALA:H | 1:GD:316:GLY:HA2 | 1.85 | 0.42 |
| 1:GD:414:LEU:HD23 | 1:GD:486:ARG:HE | 1.84 | 0.42 |
| 1:GE:158:ASN:CG | 1:GE:160:GLN:HG2 | 2.40 | 0.42 |
| 1:GE:209:TRP:O | 1:GE:210:THR:C | 2.58 | 0.42 |
| 1:GE:533:ASP:O | 1:GE:535:LEU:N | 2.53 | 0.42 |
| 1:GE:46:TYR:HB3 | 1:GE:53:LEU:HD23 | 2.02 | 0.42 |
| 1:GE:611:LEU:HD11 | 1:GE:616:PHE:CE2 | 2.55 | 0.42 |
| 1:GE:66:TYR:OH | 11:IE:57:GLU:OE1 | 2.37 | 0.42 |
| 2:GF:306:ARG:C | 2:GF:307:ILE:HD12 | 2.41 | 0.42 |
| 2:GF:412:THR:OG1 | 2:GF:413:TRP:N | 2.53 | 0.42 |
| 2:GF:618:PHE:CD1 | 2:GF:619:LEU:HB2 | 2.55 | 0.42 |
| 2:GF:967:ASP:OD1 | 2:GF:967:ASP:N | 2.53 | 0.42 |
| 3:GG:147:LEU:HD21 | 3:GG:152:GLU:HB3 | 2.02 | 0.42 |
| 3:GG:292:ALA:HB1 | 3:GG:297:TYR:CZ | 2.54 | 0.42 |
| 3:GG:96:GLY:HA2 | 3:GG:103:PRO:CB | 2.50 | 0.42 |
| 3:GH:150:LYS:HG3 | 3:GH:160:TRP:CG | 2.55 | 0.42 |
| 4:GJ:209:VAL:HG13 | 4:GJ:271:GLY:O | 2.19 | 0.42 |
| 4:H:100:ARG:NH2 | 4:H:128:ASP:OD1 | 2.53 | 0.42 |
| 4:F:15:ILE:HD13 | 4:H:25:PHE:HB2 | 2.02 | 0.42 |
| 4:HA:100:ARG:NH2 | 4:HA:128:ASP:OD1 | 2.53 | 0.42 |
| 4:HA:131:LYS:HD3 | 4:HA:161:ASN:HD22 | 1.85 | 0.42 |
| 4:GI:10:ILE:HB | 4:HA:32:ASN:HD21 | 1.85 | 0.42 |
| 5:HB:137:TYR:HA | 5:HB:143:TRP:HD1 | 1.84 | 0.42 |
| 5:HB:18:TYR:CE1 | 5:HB:20:ARG:HB3 | 2.55 | 0.42 |
| 5:HB:355:ASP:OD1 | 5:HB:356:TYR:N | 2.49 | 0.42 |
| 5:HC:169:VAL:HG13 | 5:HC:174:GLN:OE1 | 2.20 | 0.42 |
| 5:HC:341:GLU:C | 5:HC:343:SER:H | 2.22 | 0.42 |
| 5:HC:290:SER:HA | 5:HC:371:PHE:H | 1.85 | 0.42 |
| 5:HC:54:ALA:HB2 | 5:HC:71:ASN:O | 2.20 | 0.42 |
| 5:HD:264:ARG:HH12 | 6:HE:2:SER:N | 2.17 | 0.42 |
| 5:HD:322:GLY:CA | 5:HD:359:GLU:HA | 2.50 | 0.42 |
| 6:HE:88:TRP:HB3 | 6:HE:90:PHE:CE1 | 2.55 | 0.42 |
| 6:HG:109:VAL:HG13 | 6:HG:178:ILE:HG21 | 2.02 | 0.42 |
| 7:HH:251:ASN:HB2 | 7:HI:253:ARG:HH22 | 1.84 | 0.42 |
| 7:HH:288:ILE:O | 7:HI:288:ILE:N | 2.44 | 0.42 |
| 7:HH:429:CYS:HA | 7:HJ:511:GLU:OE1 | 2.20 | 0.42 |
| 7:HI:480:ARG:CZ | 7:HJ:465:ARG:HG3 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:60:ILE:HG22 | 7:HI:51:SER:C | 2.40 | 0.42 |
| 7:HI:359:TRP:CH2 | 7:HI:524:LYS:HB2 | 2.54 | 0.42 |
| 7:HI:77:THR:OG1 | 7:HI:78:PRO:HD2 | 2.19 | 0.42 |
| 7:HJ:111:ASN:ND2 | 7:HJ:114:SER:HB3 | 2.34 | 0.42 |
| 7:HH:503:ASN:HD21 | 7:HJ:446:LYS:H | 1.68 | 0.42 |
| 5:I:185:SER:HB2 | 5:I:228:PHE:HE1 | 1.84 | 0.42 |
| 5:I:382:ASN:O | 5:I:383:ILE:HD13 | 2.20 | 0.42 |
| 8:IA:88:TRP:CE3 | 8:IA:134:PRO:HD3 | 2.53 | 0.42 |
| 10:ID:312:GLY:HA2 | 10:ID:313:PRO:HA | 1.80 | 0.42 |
| 11:IE:6:PHE:HE1 | 11:IE:188:MET:O | 2.03 | 0.42 |
| 12:IF:23:SER:O | 12:IF:202:ASN:N | 2.46 | 0.42 |
| 5:J:138:CYS:SG | 5:J:140:PRO:HD2 | 2.59 | 0.42 |
| 5:J:154:ILE:HD12 | 5:J:155:THR:N | 2.35 | 0.42 |
| 5:J:328:LEU:HG | 5:J:329:PHE:H | 1.84 | 0.42 |
| 5:K:322:GLY:CA | 5:K:359:GLU:HA | 2.50 | 0.42 |
| 5:K:311:VAL:HA | 5:K:382:ASN:O | 2.20 | 0.42 |
| 5:K:264:ARG:HH12 | 6:L:2:SER:N | 2.18 | 0.42 |
| 6:L:64:ILE:HG23 | 6:L:217:ARG:HH12 | 1.84 | 0.42 |
| 6:N:88:TRP:HB3 | 6:N:90:PHE:CE1 | 2.55 | 0.42 |
| 7:O:127:ASN:O | 7:O:131:THR:HG23 | 2.20 | 0.42 |
| 7:O:183:ALA:O | 7:O:184:THR:HG23 | 2.19 | 0.42 |
| 7:O:228:ILE:HG21 | 7:O:244:ALA:HB2 | 2.01 | 0.42 |
| 7:P:480:ARG:HD3 | 7:Q:462:ASN:ND2 | 2.35 | 0.42 |
| 10:U:133:LYS:HB3 | 10:U:208:THR:O | 2.20 | 0.42 |
| 12:W:185:VAL:HG23 | 12:W:186:THR:N | 2.35 | 0.42 |
| 1:X:414:LEU:HD21 | 1:X:486:ARG:HH21 | 1.85 | 0.42 |
| 1:X:491:PHE:CE2 | 1:X:619:GLN:HA | 2.55 | 0.42 |
| 1:Y:158:ASN:ND2 | 1:Y:160:GLN:HG2 | 2.35 | 0.42 |
| 1:Y:506:LYS:O | 1:Y:509:SER:OG | 2.19 | 0.42 |
| 13:YA:209[C]:GLN:HB3 | 13:YA:211[C]:VAL:HG23 | 2.02 | 0.42 |
| 13:YA:280[F]:MET:O | 13:YA:284[F]:MET:HG2 | 2.20 | 0.42 |
| 13:YA:320[D]:THR:HG22 | 13:YA:323[D]:ARG:HB3 | 2.00 | 0.42 |
| 13:YB:321[A]:LYS:HD3 | 13:YC:452[A]:GLY:CA | 2.46 | 0.42 |
| 13:YB:453[D]:ASP:O | 13:YC:445[D]:ASP:HA | 2.20 | 0.42 |
| 13:YB:454[E]:LYS:C | 13:YB:455[E]:LYS:HG3 | 2.39 | 0.42 |
| 13:YB:566[E]:THR:HG23 | 13:YC:558[E]:SER:HA | 2.02 | 0.42 |
| 13:YB:76[D]:PRO:HG3 | 13:YB:96[D]:VAL:CB | 2.50 | 0.42 |
| 13:YB:8[D]:LEU:HD23 | 13:YB:8[D]:LEU:HA | 1.79 | 0.42 |
| 13:YC:180[E]:LEU:HA | 13:YC:180[E]:LEU:HD13 | 1.76 | 0.42 |
| 13:YC:389[D]:TYR:O | 13:YC:405[D]:ASP:HB2 | 2.19 | 0.42 |
| 13:YC:410[A]:GLU:O | 13:YC:426[A]:PRO:HA | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:439[A]:TYR:HB3 | 13:YC:441[A]:ILE:CD1 | 2.49 | 0.42 |
| 13:YC:439[E]:TYR:HB3 | 13:YC:441[E]:ILE:CD1 | 2.50 | 0.42 |
| 13:YB:450[D]:VAL:HG11 | 13:YC:446[D]:GLY:H | 1.85 | 0.42 |
| 13:YA:445[D]:ASP:HA | 13:YC:453[D]:ASP:O | 2.20 | 0.42 |
| 13:YA:463[C]:ILE:HA | 13:YC:471[C]:LEU:O | 2.20 | 0.42 |
| 13:YA:463[F]:ILE:HA | 13:YC:471[F]:LEU:O | 2.20 | 0.42 |
| 13:YA:60[B]:PRO:HB3 | 13:YC:60[B]:PRO:HB3 | 2.01 | 0.42 |
| 13:YA:75[E]:GLY:O | 13:YC:61[E]:ILE:O | 2.37 | 0.42 |
| 13:YC:66[D]:MET:HE3 | 13:YC:66[D]:MET:HA | 2.02 | 0.42 |
| 13:YC:76[B]:PRO:HB3 | 13:YC:96[B]:VAL:O | 2.20 | 0.42 |
| 14:YD:43[B]:SER:O | 14:YD:189[B]:TRP:HB2 | 2.20 | 0.42 |
| 14:YD:334[C]:LYS:HD2 | 14:YD:334[C]:LYS:HA | 1.92 | 0.42 |
| 14:YE:114[A]:SER:HA | 14:YE:167[A]:GLU:OE1 | 2.20 | 0.42 |
| 14:YE:43[D]:SER:O | 14:YE:189[D]:TRP:HB2 | 2.20 | 0.42 |
| 14:YE:17[B]:PHE:HE2 | 14:YE:26[B]:ASN:HA | 1.85 | 0.42 |
| 14:YE:290[A]:ASN:C | 14:YE:290[A]:ASN:OD1 | 2.58 | 0.42 |
| 14:YF:114[A]:SER:HA | 14:YF:167[A]:GLU:OE1 | 2.20 | 0.42 |
| 14:YF:43[F]:SER:O | 14:YF:189[F]:TRP:HB2 | 2.20 | 0.42 |
| 14:YF:212[A]:ILE:HG12 | 14:YF:228[A]:TYR:HB2 | 2.02 | 0.42 |
| 14:YF:360[F]:ASN:HD22 | 14:YF:360[F]:ASN:N | 1.98 | 0.42 |
| 2:Z:186:ASP:HB3 | 2:Z:189:ARG:HE | 1.83 | 0.42 |
| 1:A:146:VAL:HG11 | 1:A:172:ILE:HG12 | 2.01 | 0.42 |
| 1:A:270:ILE:HD13 | 1:A:270:ILE:HG21 | 1.69 | 0.42 |
| 1:A:315:GLY:HA2 | 1:A:356:ILE:CD1 | 2.50 | 0.42 |
| 4:AA:251:ASN:N | 4:AA:266:SER:O | 2.53 | 0.42 |
| 4:AA:32:ASN:HD21 | 4:AB:10:ILE:HB | 1.84 | 0.42 |
| 4:AB:44:ASP:O | 4:AB:59:GLN:NE2 | 2.52 | 0.42 |
| 5:AC:185:SER:HB2 | 5:AC:228:PHE:HE1 | 1.84 | 0.42 |
| 5:AC:424:ASP:OD2 | 5:AC:427:LYS:HB3 | 2.19 | 0.42 |
| 5:AD:117:ILE:HG13 | 5:AD:118:LYS:H | 1.85 | 0.42 |
| 5:AD:454:TYR:HD1 | 5:AD:458:THR:HG21 | 1.85 | 0.42 |
| 7:AI:176:ILE:HG12 | 7:AI:177:ALA:N | 2.33 | 0.42 |
| 7:AJ:335:ASN:OD1 | 7:AJ:336:GLU:N | 2.53 | 0.42 |
| 1:B:158:ASN:ND2 | 1:B:160:GLN:HG2 | 2.35 | 0.42 |
| 7:AI:501:THR:HB | 7:BA:422:LYS:NZ | 2.35 | 0.42 |
| 11:BF:71:TRP:O | 11:BF:74:LEU:N | 2.53 | 0.42 |
| 12:BG:187:GLY:C | 12:BG:188:LEU:HD12 | 2.41 | 0.42 |
| 12:BG:220:SER:HA | 12:BG:243:PHE:HD1 | 1.82 | 0.42 |
| 1:BH:192:ILE:HG22 | 1:BH:272:TYR:CD1 | 2.54 | 0.42 |
| 1:BH:105:ALA:HB2 | 1:BH:275:THR:HG21 | 2.02 | 0.42 |
| 1:BH:448:TYR:CE2 | 1:BH:642:PHE:HB2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BI:340:VAL:O | 1:BI:341:THR:OG1 | 2.27 | 0.42 |
| 1:BI:485:VAL:HG22 | 1:BI:624:TYR:CD1 | 2.55 | 0.42 |
| 2:BJ:146:LEU:HA | 2:BJ:585:MET:HA | 2.02 | 0.42 |
| 2:BJ:217:GLN:HG2 | 2:BJ:218:THR:H | 1.85 | 0.42 |
| 2:BJ:439:LYS:HG3 | 2:BJ:440:LEU:HD12 | 2.01 | 0.42 |
| 2:BJ:740:ILE:O | 2:BJ:743:SER:HB3 | 2.20 | 0.42 |
| 2:BJ:784:GLN:HG2 | 2:BJ:830:ARG:CB | 2.50 | 0.42 |
| 2:BJ:981:GLN:CG | 2:BJ:982:LEU:N | 2.82 | 0.42 |
| 2:C:380:ILE:HB | 2:C:396:ILE:HG21 | 2.01 | 0.42 |
| 2:C:59:LEU:HA | 2:C:59:LEU:HD23 | 1.85 | 0.42 |
| 2:C:644:ASP:HB2 | 2:C:646:ARG:HG2 | 2.01 | 0.42 |
| 2:C:906:LEU:HD12 | 2:C:907:LYS:N | 2.35 | 0.42 |
| 2:C:937:THR:HA | 2:C:941:GLU:O | 2.19 | 0.42 |
| 3:CA:282:LYS:NZ | 3:CA:287:ASP:O | 2.53 | 0.42 |
| 3:CA:292:ALA:HB1 | 3:CA:297:TYR:CZ | 2.54 | 0.42 |
| 3:CB:104:TYR:CB | 3:CB:165:ARG:HB2 | 2.49 | 0.42 |
| 4:CD:100:ARG:NH2 | 4:CD:128:ASP:OD1 | 2.53 | 0.42 |
| 4:CC:54:THR:HA | 4:CD:7:LYS:O | 2.20 | 0.42 |
| 5:CF:316:ILE:HD13 | 6:DA:7:LYS:HG3 | 2.02 | 0.42 |
| 5:CG:154:ILE:HD12 | 5:CG:155:THR:N | 2.35 | 0.42 |
| 5:CG:289:LYS:O | 5:CG:290:SER:OG | 2.25 | 0.42 |
| 5:CG:421:ASN:HB2 | 5:CG:434:GLU:CG | 2.49 | 0.42 |
| 5:CG:49:TRP:HH2 | 5:CG:96:ARG:HE | 1.67 | 0.42 |
| 5:CH:363:ASN:HD21 | 7:HJ:472:ARG:HE | 1.68 | 0.42 |
| 3:D:292:ALA:HB1 | 3:D:297:TYR:CZ | 2.54 | 0.42 |
| 6:DA:109:VAL:HG13 | 6:DA:178:ILE:HG21 | 2.02 | 0.42 |
| 7:DB:497:ASN:OD1 | 7:DB:500:TYR:N | 2.53 | 0.42 |
| 9:DG:20:ASN:C | 9:DG:20:ASN:OD1 | 2.57 | 0.42 |
| 11:DI:88:THR:O | 11:DI:163:ASN:ND2 | 2.53 | 0.42 |
| 3:E:254:ASP:CG | 3:E:256:VAL:HG12 | 2.40 | 0.42 |
| 3:E:294:LYS:HB2 | 3:E:297:TYR:CZ | 2.53 | 0.42 |
| 1:EA:111:MET:HG3 | 1:EA:111:MET:O | 2.20 | 0.42 |
| 1:EB:382:LEU:HD12 | 1:EB:647:ARG:HH12 | 1.85 | 0.42 |
| 1:EB:533:ASP:O | 1:EB:535:LEU:N | 2.53 | 0.42 |
| 2:EC:315:ASP:O | 2:EC:316:ASP:HB2 | 2.20 | 0.42 |
| 2:EC:750:VAL:HG23 | 2:EC:751:LEU:H | 1.84 | 0.42 |
| 2:EC:967:ASP:N | 2:EC:967:ASP:OD1 | 2.53 | 0.42 |
| 3:EE:300:GLU:OE1 | 3:EE:300:GLU:N | 2.44 | 0.42 |
| 4:EG:131:LYS:HD3 | 4:EG:161:ASN:HD22 | 1.85 | 0.42 |
| 5:EI:355:ASP:OD1 | 5:EI:356:TYR:N | 2.49 | 0.42 |
| 5:EI:382:ASN:O | 5:EI:383:ILE:HD13 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:EI:450:PHE:CZ | 5:EI:454:TYR:HD2 | 2.38 | 0.42 |
| 5:EI:573:LYS:HD3 | 5:EJ:537:THR:O | 2.20 | 0.42 |
| 2:EC:1001:PHE:CE2 | 5:EI:5:ILE:HD11 | 2.55 | 0.42 |
| 5:EJ:257:SER:O | 5:EJ:258:TYR:HB3 | 2.20 | 0.42 |
| 5:EJ:285:LEU:HD21 | 5:EJ:375:PHE:N | 2.21 | 0.42 |
| 5:EJ:430:TRP:HA | 5:EJ:431:PRO:C | 2.40 | 0.42 |
| 5:FA:150:GLN:HG3 | 5:FA:152:ASP:HB3 | 2.01 | 0.42 |
| 5:FA:304:ILE:HD12 | 5:FA:304:ILE:O | 2.20 | 0.42 |
| 5:FA:304:ILE:HD12 | 5:FA:306:PRO:HA | 2.02 | 0.42 |
| 5:FA:322:GLY:O | 5:FA:323:THR:OG1 | 2.34 | 0.42 |
| 5:FA:454:TYR:O | 5:FA:600:ARG:NH1 | 2.43 | 0.42 |
| 6:FC:195:LEU:HD13 | 6:FC:215:PHE:CE1 | 2.52 | 0.42 |
| 6:FC:205:ASN:HD22 | 7:HI:175:GLN:CG | 2.33 | 0.42 |
| 6:FD:71:ILE:O | 6:FD:215:PHE:N | 2.36 | 0.42 |
| 7:FE:260:ARG:HD3 | 7:FG:262:VAL:HG23 | 2.01 | 0.42 |
| 7:FE:26:PRO:HA | 7:FE:27:PRO:HD3 | 1.80 | 0.42 |
| 7:FF:228:ILE:O | 7:FG:226:GLY:N | 2.50 | 0.42 |
| 7:FE:312:GLY:N | 7:FF:316:THR:O | 2.39 | 0.42 |
| 7:FF:358:ALA:HB1 | 7:FF:524:LYS:HE3 | 2.02 | 0.42 |
| 7:FE:472:ARG:NH1 | 7:FG:474:GLY:HA2 | 2.34 | 0.42 |
| 7:FG:77:THR:OG1 | 7:FG:78:PRO:HD2 | 2.20 | 0.42 |
| 4:G:43:GLY:HA2 | 4:G:62:HIS:CE1 | 2.55 | 0.42 |
| 11:GB:74:LEU:HD12 | 11:GB:74:LEU:HA | 1.78 | 0.42 |
| 1:GD:178:ILE:HA | 1:GD:178:ILE:HD12 | 1.84 | 0.42 |
| 1:GD:361:GLN:HE21 | 1:GD:456:ASN:HB2 | 1.84 | 0.42 |
| 1:GD:609:ILE:HG22 | 1:GD:611:LEU:HG | 2.01 | 0.42 |
| 1:GD:90:VAL:HG11 | 1:GD:228:GLU:HG2 | 2.01 | 0.42 |
| 1:GE:377:LYS:HB3 | 1:GE:377:LYS:HE2 | 1.65 | 0.42 |
| 1:GE:66:TYR:O | 1:GE:70:PHE:N | 2.41 | 0.42 |
| 1:GD:67:ILE:HD11 | 1:GE:67:ILE:HG21 | 2.01 | 0.42 |
| 3:E:176:ALA:HB3 | 2:GF:508:TYR:HA | 2.02 | 0.42 |
| 2:GF:516:TRP:HE1 | 2:GF:518:LYS:HG2 | 1.85 | 0.42 |
| 2:GF:21:VAL:HG23 | 2:GF:69:PHE:HB3 | 2.02 | 0.42 |
| 3:GH:268:GLY:HA3 | 3:GH:318:ILE:O | 2.20 | 0.42 |
| 4:GI:161:ASN:HB3 | 4:HA:168:PHE:CE1 | 2.55 | 0.42 |
| 4:GI:233:SER:OG | 4:HA:236:ALA:HA | 2.20 | 0.42 |
| 4:GI:190:PRO:HA | 4:GI:262:THR:HA | 2.01 | 0.42 |
| 4:HA:44:ASP:O | 4:HA:59:GLN:NE2 | 2.52 | 0.42 |
| 5:HB:193:VAL:O | 5:HB:199:GLU:N | 2.46 | 0.42 |
| 5:HB:181:PHE:HE2 | 5:HB:246:THR:HG22 | 1.83 | 0.42 |
| 5:HB:265:LEU:HD22 | 5:HB:281:TYR:HD2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:321:ALA:O | 5:HB:324:VAL:HG12 | 2.19 | 0.42 |
| 5:HB:322:GLY:N | 5:HB:360:THR:HG23 | 2.35 | 0.42 |
| 5:HB:382:ASN:O | 5:HB:383:ILE:HD13 | 2.20 | 0.42 |
| 5:HC:138:CYS:SG | 5:HC:140:PRO:HD2 | 2.60 | 0.42 |
| 5:HC:154:ILE:HD12 | 5:HC:155:THR:N | 2.35 | 0.42 |
| 5:HC:48:ALA:C | 5:HC:49:TRP:CD1 | 2.93 | 0.42 |
| 5:HD:311:VAL:HA | 5:HD:382:ASN:O | 2.20 | 0.42 |
| 5:HB:418:GLY:C | 5:HD:472:TYR:HB3 | 2.41 | 0.42 |
| 6:HE:109:VAL:HG13 | 6:HE:178:ILE:HG21 | 2.02 | 0.42 |
| 6:HE:90:PHE:O | 6:HE:154:SER:HB2 | 2.19 | 0.42 |
| 6:HE:195:LEU:HA | 6:HE:215:PHE:HD1 | 1.85 | 0.42 |
| 6:HF:88:TRP:HB3 | 6:HF:90:PHE:CE1 | 2.55 | 0.42 |
| 6:HF:10:VAL:CA | 6:HG:13:ARG:HD2 | 2.35 | 0.42 |
| 6:HG:90:PHE:O | 6:HG:154:SER:HB2 | 2.19 | 0.42 |
| 7:HH:78:PRO:HB2 | 7:HI:69:GLY:HA2 | 2.01 | 0.42 |
| 7:HI:358:ALA:HB1 | 7:HI:524:LYS:HE3 | 2.02 | 0.42 |
| 5:HC:200:LEU:HB2 | 7:HI:5:THR:HG21 | 2.01 | 0.42 |
| 7:HH:99:ARG:N | 7:HI:95:TYR:HD1 | 2.18 | 0.42 |
| 7:HH:39:ILE:HG22 | 7:HJ:44:VAL:CG2 | 2.49 | 0.42 |
| 12:IF:18:ARG:HB2 | 12:IF:21:MET:HG2 | 2.01 | 0.42 |
| 5:J:139:ALA:HB3 | 5:J:140:PRO:HD3 | 2.01 | 0.42 |
| 5:J:169:VAL:HG13 | 5:J:174:GLN:OE1 | 2.20 | 0.42 |
| 5:J:215:PRO:HB3 | 5:J:229:ASN:C | 2.39 | 0.42 |
| 5:J:305:ASN:HB3 | 5:K:255:ARG:HH12 | 1.85 | 0.42 |
| 5:I:590:GLN:O | 5:J:521:GLY:HA3 | 2.20 | 0.42 |
| 5:K:316:ILE:HD11 | 6:L:7:LYS:NZ | 2.35 | 0.42 |
| 5:K:507:ASP:OD1 | 5:K:510:GLY:N | 2.53 | 0.42 |
| 6:L:82:VAL:HG23 | 6:L:187:LYS:HE3 | 2.02 | 0.42 |
| 7:O:102:THR:O | 7:O:105:GLU:N | 2.52 | 0.42 |
| 7:O:182:THR:OG1 | 7:O:190:VAL:O | 2.30 | 0.42 |
| 7:O:425:LEU:HD11 | 7:P:505:PRO:O | 2.20 | 0.42 |
| 7:O:470:GLY:O | 7:Q:476:ASP:N | 2.52 | 0.42 |
| 7:O:473:LYS:HE2 | 5:FA:362:GLU:CD | 2.39 | 0.42 |
| 7:O:503:ASN:ND2 | 7:Q:445:HIS:HB2 | 2.35 | 0.42 |
| 7:O:60:ILE:HG22 | 7:P:51:SER:C | 2.41 | 0.42 |
| 7:P:515:TRP:CE3 | 7:Q:439:ILE:HA | 2.55 | 0.42 |
| 7:Q:405:ARG:HB2 | 7:Q:430:THR:OG1 | 2.20 | 0.42 |
| 1:A:46:TYR:HE1 | 9:T:17:MET:HB2 | 1.84 | 0.42 |
| 10:U:62:LEU:O | 10:U:128:LEU:HD12 | 2.20 | 0.42 |
| 12:W:171:TYR:HD1 | 12:W:239:PHE:CE2 | 2.38 | 0.42 |
| 12:W:225:ALA:HB1 | 12:W:226:PRO:HD2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:360:VAL:HG23 | 1:X:375:ALA:O | 2.20 | 0.42 |
| 1:X:655:LEU:HD12 | 1:X:655:LEU:O | 2.19 | 0.42 |
| 13:YA:180[C]:LEU:HA | 13:YA:180[C]:LEU:HD13 | 1.75 | 0.42 |
| 13:YA:293[E]:ASN:HA | 13:YA:296[E]:LEU:HB2 | 2.01 | 0.42 |
| 13:YA:330[B]:ILE:HD12 | 13:YA:336[B]:LEU:HD12 | 2.01 | 0.42 |
| 13:YA:373[D]:ARG:HA | 13:YA:373[D]:ARG:NE | 2.30 | 0.42 |
| 13:YA:459[A]:GLY:N | 13:YB:450[A]:VAL:O | 2.53 | 0.42 |
| 13:YA:459[D]:GLY:N | 13:YB:450[D]:VAL:O | 2.53 | 0.42 |
| 13:YA:38[A]:GLN:O | 13:YA:46[A]:GLY:HA2 | 2.20 | 0.42 |
| 13:YA:538[A]:VAL:O | 13:YC:546[A]:VAL:HA | 2.19 | 0.42 |
| 13:YA:61[F]:ILE:HB | 13:YB:75[F]:GLY:CA | 2.41 | 0.42 |
| 13:YA:66[E]:MET:HA | 13:YA:66[E]:MET:HE3 | 2.02 | 0.42 |
| 13:YB:132[D]:LEU:O | 13:YB:390[D]:VAL:HG11 | 2.19 | 0.42 |
| 13:YB:209[A]:GLN:HB3 | 13:YB:211[A]:VAL:HG23 | 2.02 | 0.42 |
| 13:YB:277[A]:LEU:HD23 | 13:YB:277[A]:LEU:HA | 1.80 | 0.42 |
| 13:YB:277[B]:LEU:HA | 13:YB:277[B]:LEU:HD23 | 1.79 | 0.42 |
| 13:YB:293[A]:ASN:HA | 13:YB:296[A]:LEU:HB2 | 2.01 | 0.42 |
| 13:YB:439[B]:TYR:HB3 | 13:YB:441[B]:ILE:CD1 | 2.50 | 0.42 |
| 13:YB:450[E]:VAL:HG11 | 13:YC:446[E]:GLY:H | 1.85 | 0.42 |
| 13:YB:453[A]:ASP:O | 13:YC:445[A]:ASP:HA | 2.20 | 0.42 |
| 13:YB:506[C]:VAL:HG21 | 13:YC:502[C]:VAL:HG21 | 2.02 | 0.42 |
| 13:YB:530[F]:VAL:HG22 | 13:YC:522[F]:VAL:HG13 | 2.01 | 0.42 |
| 13:YB:61[A]:ILE:CG2 | 13:YC:60[A]:PRO:HD3 | 2.50 | 0.42 |
| 13:YB:61[D]:ILE:CG2 | 13:YC:60[D]:PRO:HD3 | 2.50 | 0.42 |
| 13:YB:459[D]:GLY:N | 13:YC:450[D]:VAL:O | 2.45 | 0.42 |
| 13:YA:538[C]:VAL:O | 13:YC:546[C]:VAL:HA | 2.19 | 0.42 |
| 13:YC:552[F]:GLU:HB2 | 13:YC:554[F]:MET:HE1 | 2.02 | 0.42 |
| 13:YA:550[E]:TRP:HB2 | 13:YC:554[E]:MET:HG3 | 2.02 | 0.42 |
| 13:YC:66[B]:MET:HE3 | 13:YC:66[B]:MET:HA | 2.01 | 0.42 |
| 13:YC:66[A]:MET:HE3 | 13:YC:66[A]:MET:HA | 2.02 | 0.42 |
| 14:YD:124[E]:PHE:CZ | 14:YD:135[E]:MET:HG2 | 2.55 | 0.42 |
| 14:YD:114[C]:SER:HA | 14:YD:167[C]:GLU:OE1 | 2.20 | 0.42 |
| 14:YD:43[D]:SER:O | 14:YD:189[D]:TRP:HB2 | 2.20 | 0.42 |
| 14:YD:290[B]:ASN:C | 14:YD:290[B]:ASN:OD1 | 2.58 | 0.42 |
| 14:YD:238[C]:THR:N | 14:YD:307[C]:TYR:O | 2.52 | 0.42 |
| 14:YD:373[A]:LYS:HE2 | 14:YD:373[A]:LYS:HB3 | 1.89 | 0.42 |
| 14:YE:112[D]:ILE:HB | 14:YE:140[D]:TYR:OH | 2.19 | 0.42 |
| 14:YE:210[A]:PRO:HB2 | 14:YE:228[A]:TYR:CD2 | 2.55 | 0.42 |
| 13:YB:24[B]:LEU:HD23 | 14:YE:259[B]:LEU:CD2 | 2.49 | 0.42 |
| 13:YB:24[D]:LEU:HD23 | 14:YE:259[D]:LEU:CD2 | 2.50 | 0.42 |
| 14:YE:290[C]:ASN:OD1 | 14:YE:290[C]:ASN:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:330[E]:LYS:HG2 | 14:YF:101[E]:GLY:HA3 | 2.02 | 0.42 |
| 14:YF:124[B]:PHE:CZ | 14:YF:135[B]:MET:HG2 | 2.55 | 0.42 |
| 14:YF:124[C]:PHE:CZ | 14:YF:135[C]:MET:HG2 | 2.55 | 0.42 |
| 14:YF:172[B]:TYR:CZ | 14:YF:176[B]:VAL:HG21 | 2.55 | 0.42 |
| 14:YF:210[E]:PRO:HB2 | 14:YF:228[E]:TYR:CD2 | 2.55 | 0.42 |
| 14:YF:210[F]:PRO:HB2 | 14:YF:228[F]:TYR:CD2 | 2.55 | 0.42 |
| 14:YD:91[D]:LYS:O | 14:YF:242[D]:PRO:HD2 | 2.20 | 0.42 |
| 14:YF:290[A]:ASN:OD1 | 14:YF:290[A]:ASN:C | 2.58 | 0.42 |
| 14:YF:290[B]:ASN:OD1 | 14:YF:290[B]:ASN:C | 2.58 | 0.42 |
| 14:YF:290[D]:ASN:C | 14:YF:290[D]:ASN:OD1 | 2.58 | 0.42 |
| 14:YF:47[D]:ARG:NH1 | 14:YF:341[D]:GLU:OE1 | 2.53 | 0.42 |
| 14:YF:75[E]:ALA:HB2 | 14:YF:83[E]:VAL:HA | 2.01 | 0.42 |
| 14:YE:242[B]:PRO:HD2 | 14:YF:91[B]:LYS:O | 2.20 | 0.42 |
| 2:Z:217:GLN:HG2 | 2:Z:218:THR:H | 1.85 | 0.42 |
| 2:Z:28:VAL:HG23 | 2:Z:29:GLY:N | 2.35 | 0.42 |
| 2:Z:450:PHE:HE2 | 2:Z:473:TYR:HH | 1.66 | 0.42 |
| 2:Z:580:LYS:HG2 | 2:Z:581:TYR:N | 2.22 | 0.42 |
| 2:Z:921:TRP:N | 2:Z:921:TRP:CD1 | 2.85 | 0.42 |
| 1:A:167:LEU:HD23 | 1:A:167:LEU:HA | 1.76 | 0.41 |
| 1:A:472:ASP:O | 1:A:473:HIS:CG | 2.73 | 0.41 |
| 1:A:510:MET:HE1 | 1:A:623:LEU:HD21 | 2.01 | 0.41 |
| 5:AC:460:TYR:CE1 | 5:AD:458:THR:HG23 | 2.54 | 0.41 |
| 5:AC:558:ASP:O | 5:AC:566:TYR:HE2 | 2.02 | 0.41 |
| 5:AD:154:ILE:HD12 | 5:AD:155:THR:N | 2.35 | 0.41 |
| 5:AD:186:TYR:CE1 | 5:AD:246:THR:HA | 2.50 | 0.41 |
| 5:AD:290:SER:HA | 5:AD:371:PHE:H | 1.85 | 0.41 |
| 5:AD:34:TYR:OH | 5:AD:41:ASP:C | 2.58 | 0.41 |
| 5:AD:267:ASP:H | 5:AD:377:HIS:HB2 | 1.84 | 0.41 |
| 5:AD:542:LEU:HD11 | 5:AE:569:TYR:HE2 | 1.82 | 0.41 |
| 5:AE:192:ARG:CG | 5:AE:245:GLU:HB2 | 2.50 | 0.41 |
| 5:AE:320:LEU:HG | 5:AE:357:SER:CB | 2.49 | 0.41 |
| 6:AG:217:ARG:HE | 6:AG:219:ALA:C | 2.23 | 0.41 |
| 6:AH:195:LEU:HD13 | 6:AH:215:PHE:CE1 | 2.52 | 0.41 |
| 7:AI:161:THR:H | 7:AI:164:LYS:HZ1 | 1.68 | 0.41 |
| 7:AI:190:VAL:HB | 7:AJ:189:GLY:N | 2.35 | 0.41 |
| 1:B:65:LEU:HD21 | 11:V:70:TYR:OH | 2.20 | 0.41 |
| 8:BB:89:GLN:HB3 | 8:BB:134:PRO:CG | 2.50 | 0.41 |
| 8:BC:15:PHE:N | 8:BC:15:PHE:CD1 | 2.84 | 0.41 |
| 9:BD:47:ARG:HD2 | 9:BD:47:ARG:HA | 1.79 | 0.41 |
| 12:BG:15:ASP:O | 12:BG:16:PHE:CD1 | 2.73 | 0.41 |
| 12:BG:18:ARG:HB2 | 12:BG:21:MET:HG2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BH:111:MET:HG3 | 1:BH:111:MET:O | 2.20 | 0.41 |
| 1:BH:123:ILE:HA | 1:BH:123:ILE:HD12 | 1.77 | 0.41 |
| 1:BH:209:TRP:HD1 | 1:BH:225:TYR:CE1 | 2.35 | 0.41 |
| 1:BH:201:VAL:HG21 | 1:BH:262:PRO:HB3 | 2.02 | 0.41 |
| 1:BH:433:GLU:OE2 | 1:BH:655:LEU:HD11 | 2.20 | 0.41 |
| 1:BH:361:GLN:HE21 | 1:BH:456:ASN:HB2 | 1.84 | 0.41 |
| 1:BH:377:LYS:HD3 | 1:BH:641:VAL:HG21 | 2.02 | 0.41 |
| 1:BI:382:LEU:HD12 | 1:BI:647:ARG:HH12 | 1.85 | 0.41 |
| 1:BI:55:VAL:HG21 | 2:BJ:657:TYR:CZ | 2.55 | 0.41 |
| 1:BI:565:GLU:OE1 | 1:BI:571:PRO:HD3 | 2.20 | 0.41 |
| 1:BI:611:LEU:HD11 | 1:BI:616:PHE:CE2 | 2.54 | 0.41 |
| 2:BJ:21:VAL:HG23 | 2:BJ:69:PHE:HB3 | 2.02 | 0.41 |
| 2:BJ:431:TYR:HB3 | 2:BJ:485:TYR:OH | 2.20 | 0.41 |
| 2:BJ:967:ASP:N | 2:BJ:967:ASP:OD1 | 2.53 | 0.41 |
| 2:C:315:ASP:O | 2:C:316:ASP:HB2 | 2.20 | 0.41 |
| 2:C:516:TRP:HE1 | 2:C:518:LYS:HG2 | 1.85 | 0.41 |
| 2:C:139:ASN:HA | 2:C:555:ARG:NH2 | 2.34 | 0.41 |
| 2:C:21:VAL:HG23 | 2:C:69:PHE:HB3 | 2.02 | 0.41 |
| 3:CA:114:CYS:HA | 3:CA:120:ASN:HD21 | 1.85 | 0.41 |
| 3:CA:138:ASP:HA | 3:CA:150:LYS:HE3 | 2.02 | 0.41 |
| 3:CA:147:LEU:HD21 | 3:CA:152:GLU:HB3 | 2.02 | 0.41 |
| 3:CA:316:PRO:HG2 | 3:CB:6:VAL:HG13 | 2.02 | 0.41 |
| 5:CF:170:GLU:O | 5:CF:171:VAL:HG12 | 2.19 | 0.41 |
| 5:CF:18:TYR:CE1 | 5:CF:20:ARG:HB3 | 2.55 | 0.41 |
| 5:CF:382:ASN:O | 5:CF:383:ILE:HD13 | 2.20 | 0.41 |
| 5:CF:67:SER:HA | 5:CF:94:ARG:O | 2.20 | 0.41 |
| 5:CG:303:PRO:HD2 | 5:CG:365:ILE:HD13 | 2.02 | 0.41 |
| 5:CG:395:THR:OG1 | 5:CG:396:LYS:N | 2.52 | 0.41 |
| 5:CH:89:TYR:HA | 5:CH:137:TYR:CD2 | 2.55 | 0.41 |
| 5:CH:169:VAL:O | 5:CH:238:ILE:HA | 2.19 | 0.41 |
| 5:CH:304:ILE:HG21 | 5:CH:309:LEU:HG | 2.02 | 0.41 |
| 6:CI:19:GLY:H | 6:CJ:13:ARG:CZ | 2.31 | 0.41 |
| 3:D:254:ASP:HB3 | 3:D:257:TYR:CD2 | 2.55 | 0.41 |
| 7:DB:212:PRO:HA | 7:DB:215:PHE:HB3 | 2.02 | 0.41 |
| 7:DB:77:THR:HG23 | 7:DB:79:ALA:H | 1.85 | 0.41 |
| 7:DC:12:GLU:CG | 7:DC:15:TYR:H | 2.31 | 0.41 |
| 7:DB:445:HIS:NE2 | 7:DC:447:HIS:CE1 | 2.85 | 0.41 |
| 7:DC:451:PHE:HD1 | 7:DC:469:VAL:HG13 | 1.84 | 0.41 |
| 7:DD:20:PRO:CG | 7:DD:29:ILE:HG13 | 2.48 | 0.41 |
| 8:DF:25:ILE:O | 8:DF:26:SER:HB3 | 2.20 | 0.41 |
| 12:DJ:187:GLY:C | 12:DJ:188:LEU:HD12 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:192:ILE:HG22 | 1:EA:272:TYR:CD1 | 2.54 | 0.41 |
| 1:EA:328:LEU:HD23 | 1:EA:328:LEU:HA | 1.71 | 0.41 |
| 1:EA:377:LYS:HD3 | 1:EA:641:VAL:HG21 | 2.02 | 0.41 |
| 1:EB:213:SER:HA | 2:EC:733:ASP:CG | 2.40 | 0.41 |
| 1:EB:348:PHE:HZ | 1:EB:399:TYR:HD2 | 1.65 | 0.41 |
| 2:EC:29:GLY:HA2 | 3:EE:60:TYR:HB3 | 2.02 | 0.41 |
| 2:EC:618:PHE:CD1 | 2:EC:619:LEU:HB2 | 2.55 | 0.41 |
| 2:EC:683:TYR:O | 2:EC:686:LEU:N | 2.53 | 0.41 |
| 3:ED:96:GLY:HA2 | 3:ED:103:PRO:CB | 2.50 | 0.41 |
| 3:ED:248:ARG:HA | 3:ED:330:ILE:O | 2.20 | 0.41 |
| 3:ED:86:LEU:HD23 | 3:ED:86:LEU:HA | 1.68 | 0.41 |
| 3:EE:235:ASP:O | 3:EE:236:PHE:HB2 | 2.20 | 0.41 |
| 4:EH:100:ARG:NH2 | 4:EH:128:ASP:OD1 | 2.53 | 0.41 |
| 5:EI:118:LYS:HA | 5:EI:142:ARG:NH2 | 2.35 | 0.41 |
| 5:EI:18:TYR:CE1 | 5:EI:20:ARG:HB3 | 2.55 | 0.41 |
| 5:EI:304:ILE:HG12 | 5:EI:305:ASN:O | 2.20 | 0.41 |
| 5:EJ:186:TYR:HB3 | 5:EJ:227:GLY:O | 2.20 | 0.41 |
| 4:F:43:GLY:HA2 | 4:F:62:HIS:CE1 | 2.55 | 0.41 |
| 5:FA:215:PRO:HB3 | 5:FA:229:ASN:C | 2.40 | 0.41 |
| 6:FB:141:THR:HG22 | 6:FD:43:LEU:HD11 | 2.02 | 0.41 |
| 6:FB:69:THR:HA | 6:FC:73:ASN:HB3 | 2.01 | 0.41 |
| 6:FD:135:GLU:O | 6:FD:139:SER:N | 2.27 | 0.41 |
| 7:FE:141:VAL:HG23 | 7:FF:140:GLY:O | 2.20 | 0.41 |
| 7:FF:262:VAL:CG2 | 7:FG:260:ARG:HB3 | 2.50 | 0.41 |
| 7:FE:399:PHE:CE2 | 7:FG:514:PRO:HG2 | 2.55 | 0.41 |
| 4:G:100:ARG:NH2 | 4:G:128:ASP:OD1 | 2.53 | 0.41 |
| 11:GB:146:TYR:HE2 | 11:GB:150:LEU:HD23 | 1.85 | 0.41 |
| 11:GB:6:PHE:HE1 | 11:GB:188:MET:O | 2.03 | 0.41 |
| 12:GC:5:GLU:O | 12:GC:9:ASN:N | 2.41 | 0.41 |
| 1:GD:222:THR:C | 1:GD:223:ILE:HG12 | 2.40 | 0.41 |
| 1:GD:275:THR:OG1 | 1:GD:275:THR:O | 2.36 | 0.41 |
| 1:GE:62:TYR:CZ | 1:GE:66:TYR:HE2 | 2.38 | 0.41 |
| 2:GF:222:VAL:HG12 | 2:GF:224:LEU:HB2 | 2.01 | 0.41 |
| 2:GF:300:LEU:N | 2:GF:301:PRO:HD3 | 2.35 | 0.41 |
| 2:GF:315:ASP:O | 2:GF:316:ASP:HB2 | 2.20 | 0.41 |
| 2:GF:73:ASP:HB3 | 2:GF:76:THR:HG21 | 2.02 | 0.41 |
| 1:GE:403:PRO:HB2 | 2:GF:888:PHE:CD2 | 2.55 | 0.41 |
| 2:GF:947:VAL:HB | 3:GG:119:TYR:HB3 | 2.01 | 0.41 |
| 2:GF:986:ARG:HH12 | 3:GG:323:ASP:HB2 | 1.85 | 0.41 |
| 3:GG:248:ARG:HA | 3:GG:330:ILE:O | 2.20 | 0.41 |
| 3:GH:254:ASP:CG | 3:GH:256:VAL:HG12 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:GI:54:THR:HA | 4:GJ:7:LYS:O | 2.19 | 0.41 |
| 4:GJ:216:THR:CG2 | 4:HA:222:LEU:HD13 | 2.50 | 0.41 |
| 4:GI:83:THR:HA | 4:HA:63:ALA:HB3 | 2.02 | 0.41 |
| 5:HB:204:ASP:OD1 | 5:HB:205:VAL:N | 2.50 | 0.41 |
| 5:HB:472:TYR:O | 5:HC:416:ILE:HD12 | 2.20 | 0.41 |
| 5:HB:560:ASP:HB3 | 5:HB:561:GLU:H | 1.66 | 0.41 |
| 5:HC:186:TYR:HB3 | 5:HC:227:GLY:O | 2.20 | 0.41 |
| 5:HC:454:TYR:HD1 | 5:HC:458:THR:HG21 | 1.85 | 0.41 |
| 5:HD:117:ILE:HG22 | 5:HD:143:TRP:HB2 | 2.02 | 0.41 |
| 5:HD:150:GLN:HG3 | 5:HD:152:ASP:HB3 | 2.01 | 0.41 |
| 5:HD:181:PHE:HE2 | 5:HD:246:THR:HG22 | 1.85 | 0.41 |
| 7:P:195:THR:HG21 | 6:HG:32:ARG:HD3 | 2.01 | 0.41 |
| 7:HH:146:SER:N | 7:HH:149:GLN:HB2 | 2.35 | 0.41 |
| 7:HH:255:SER:N | 7:HH:278:SER:OG | 2.53 | 0.41 |
| 7:HH:77:THR:CG2 | 7:HH:80:THR:H | 2.33 | 0.41 |
| 7:HI:183:ALA:HB2 | 7:HI:189:GLY:O | 2.20 | 0.41 |
| 7:HI:255:SER:HB2 | 7:HI:261:GLY:O | 2.20 | 0.41 |
| 3:D:201:ASN:OD1 | 5:I:10:VAL:HG21 | 2.19 | 0.41 |
| 5:I:222:LEU:HD11 | 5:I:224:PRO:HD2 | 2.01 | 0.41 |
| 5:I:258:TYR:CE1 | 5:I:384:THR:HG23 | 2.55 | 0.41 |
| 5:I:450:PHE:CZ | 5:I:454:TYR:HD2 | 2.38 | 0.41 |
| 5:I:584:THR:O | 5:J:531:ASN:ND2 | 2.45 | 0.41 |
| 9:IC:64:ASN:O | 9:IC:69:THR:HG21 | 2.19 | 0.41 |
| 10:ID:133:LYS:HB3 | 10:ID:208:THR:O | 2.20 | 0.41 |
| 11:IE:88:THR:O | 11:IE:163:ASN:ND2 | 2.53 | 0.41 |
| 12:IF:124:MET:HG3 | 12:IF:170:ASN:ND2 | 2.35 | 0.41 |
| 12:IF:171:TYR:HD1 | 12:IF:239:PHE:CE2 | 2.38 | 0.41 |
| 12:IF:225:ALA:HB1 | 12:IF:226:PRO:HD2 | 2.02 | 0.41 |
| 5:J:102:TRP:HE3 | 5:J:131:SER:HB2 | 1.84 | 0.41 |
| 5:J:344:VAL:O | 5:J:345:LEU:HD12 | 2.20 | 0.41 |
| 5:K:151:ILE:HG23 | 5:K:152:ASP:N | 2.34 | 0.41 |
| 5:K:180:VAL:HG22 | 5:K:181:PHE:H | 1.84 | 0.41 |
| 6:M:7:LYS:HD3 | 6:N:11:ILE:HA | 2.01 | 0.41 |
| 7:P:146:SER:HB2 | 7:P:149:GLN:HG2 | 2.01 | 0.41 |
| 7:P:183:ALA:HB2 | 7:P:189:GLY:O | 2.20 | 0.41 |
| 7:P:190:VAL:HG12 | 7:Q:190:VAL:HG13 | 2.02 | 0.41 |
| 7:P:205:ARG:HH12 | 6:HE:218:THR:CB | 2.32 | 0.41 |
| 7:O:312:GLY:N | 7:P:316:THR:O | 2.40 | 0.41 |
| 7:P:212:PRO:CB | 7:Q:199:VAL:HA | 2.43 | 0.41 |
| 7:P:516:ASN:OD1 | 7:Q:438:GLN:HB2 | 2.19 | 0.41 |
| 7:Q:467:ASN:OD1 | 5:EJ:412:PRO:HB3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:R:91:ILE:HG22 | 8:R:107:TYR:HB3 | 2.02 | 0.41 |
| 12:W:220:SER:HA | 12:W:243:PHE:HD1 | 1.82 | 0.41 |
| 1:X:222:THR:C | 1:X:223:ILE:HG12 | 2.40 | 0.41 |
| 1:X:392:ILE:HG23 | 1:X:408:ILE:HD12 | 2.01 | 0.41 |
| 1:X:414:LEU:HD23 | 1:X:486:ARG:HE | 1.85 | 0.41 |
| 1:X:472:ASP:O | 1:X:473:HIS:CG | 2.73 | 0.41 |
| 1:Y:148:ARG:HG2 | 1:Y:149:GLU:HG3 | 2.01 | 0.41 |
| 1:Y:378:PRO:O | 1:Y:379:LYS:HG2 | 2.19 | 0.41 |
| 13:YA:280[A]:MET:O | 13:YA:284[A]:MET:HG2 | 2.19 | 0.41 |
| 13:YA:280[C]:MET:O | 13:YA:284[C]:MET:HG2 | 2.20 | 0.41 |
| 13:YA:410[A]:GLU:O | 13:YA:426[A]:PRO:HA | 2.20 | 0.41 |
| 13:YA:410[F]:GLU:O | 13:YA:426[F]:PRO:HA | 2.20 | 0.41 |
| 13:YA:439[E]:TYR:HB3 | 13:YA:441[E]:ILE:CD1 | 2.50 | 0.41 |
| 13:YA:530[C]:VAL:O | 13:YC:538[C]:VAL:HA | 2.20 | 0.41 |
| 13:YA:530[D]:VAL:O | 13:YC:538[D]:VAL:HA | 2.19 | 0.41 |
| 13:YA:550[A]:TRP:HB2 | 13:YC:554[A]:MET:HG3 | 2.02 | 0.41 |
| 13:YA:552[D]:GLU:HB2 | 13:YA:554[D]:MET:HE1 | 2.02 | 0.41 |
| 13:YA:569[B]:GLY:HA2 | 13:YB:561[B]:SER:O | 2.19 | 0.41 |
| 13:YA:66[B]:MET:HA | 13:YA:66[B]:MET:HE3 | 2.02 | 0.41 |
| 13:YA:66[C]:MET:HE3 | 13:YA:66[C]:MET:HA | 2.01 | 0.41 |
| 13:YA:76[E]:PRO:HB3 | 13:YA:98[E]:GLY:C | 2.40 | 0.41 |
| 13:YB:154[A]:THR:H | 13:YB:182[A]:ARG:NH2 | 2.17 | 0.41 |
| 13:YB:219[C]:LYS:HE3 | 13:YB:219[C]:LYS:HB2 | 1.81 | 0.41 |
| 13:YB:410[D]:GLU:O | 13:YB:426[D]:PRO:HA | 2.20 | 0.41 |
| 13:YB:436[B]:ASP:HB3 | 13:YC:429[B]:ARG:HA | 2.03 | 0.41 |
| 13:YB:442[C]:THR:HB | 13:YC:434[C]:THR:HB | 2.01 | 0.41 |
| 13:YB:506[A]:VAL:HG21 | 13:YC:502[A]:VAL:HG21 | 2.02 | 0.41 |
| 13:YB:506[B]:VAL:HG21 | 13:YC:502[B]:VAL:HG21 | 2.02 | 0.41 |
| 13:YB:552[A]:GLU:HB2 | 13:YB:554[A]:MET:HE1 | 2.01 | 0.41 |
| 13:YC:293[D]:ASN:HA | 13:YC:296[D]:LEU:HB2 | 2.01 | 0.41 |
| 13:YC:293[B]:ASN:HA | 13:YC:296[B]:LEU:HB2 | 2.01 | 0.41 |
| 13:YC:304[B]:TRP:O | 13:YC:308[B]:TYR:N | 2.33 | 0.41 |
| 13:YC:410[C]:GLU:O | 13:YC:426[C]:PRO:HA | 2.20 | 0.41 |
| 13:YA:463[D]:ILE:HA | 13:YC:471[D]:LEU:O | 2.20 | 0.41 |
| 13:YC:47[A]:ILE:HG23 | 14:YF:123[A]:PRO:CG | 2.47 | 0.41 |
| 13:YB:546[E]:VAL:HG11 | 13:YC:542[E]:VAL:HG13 | 2.00 | 0.41 |
| 13:YC:83[F]:TYR:OH | 13:YC:85[F]:HIS:HE1 | 2.03 | 0.41 |
| 14:YD:124[C]:PHE:CZ | 14:YD:135[C]:MET:HG2 | 2.55 | 0.41 |
| 14:YD:210[F]:PRO:HB2 | 14:YD:228[F]:TYR:CD2 | 2.55 | 0.41 |
| 14:YD:290[E]:ASN:OD1 | 14:YD:290[E]:ASN:C | 2.58 | 0.41 |
| 14:YD:355[C]:LEU:HA | 14:YD:355[C]:LEU:HD23 | 1.87 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:364[C]:LEU:HA | 14:YD:364[C]:LEU:HD22 | 1.79 | 0.41 |
| 14:YE:114[C]:SER:HA | 14:YE:167[C]:GLU:OE1 | 2.20 | 0.41 |
| 14:YE:172[F]:TYR:CZ | 14:YE:176[F]:VAL:HG21 | 2.54 | 0.41 |
| 14:YE:43[A]:SER:O | 14:YE:189[A]:TRP:HB2 | 2.20 | 0.41 |
| 14:YE:290[F]:ASN:OD1 | 14:YE:290[F]:ASN:C | 2.58 | 0.41 |
| 14:YE:360[B]:ASN:N | 14:YE:360[B]:ASN:HD22 | 1.98 | 0.41 |
| 14:YF:124[D]:PHE:CZ | 14:YF:135[D]:MET:HG2 | 2.55 | 0.41 |
| 14:YF:43[C]:SER:O | 14:YF:189[C]:TRP:HB2 | 2.20 | 0.41 |
| 13:YA:81[C]:ARG:HD3 | 14:YF:261[C]:SER:HA | 2.02 | 0.41 |
| 14:YF:238[E]:THR:N | 14:YF:307[E]:TYR:O | 2.53 | 0.41 |
| 14:YF:345[D]:GLU:HB3 | 14:YF:352[D]:VAL:HG13 | 2.02 | 0.41 |
| 14:YF:364[E]:LEU:HA | 14:YF:364[E]:LEU:HD22 | 1.79 | 0.41 |
| 14:YF:47[E]:ARG:NH1 | 14:YF:341[E]:GLU:OE1 | 2.53 | 0.41 |
| 2:Z:457:ASN:O | 2:Z:458:ASP:C | 2.58 | 0.41 |
| 2:Z:516:TRP:HE1 | 2:Z:518:LYS:HG2 | 1.85 | 0.41 |
| 1:A:105:ALA:HB2 | 1:A:275:THR:HG21 | 2.02 | 0.41 |
| 4:AA:43:GLY:HA2 | 4:AA:62:HIS:CE1 | 2.55 | 0.41 |
| 5:AC:322:GLY:N | 5:AC:360:THR:HG23 | 2.35 | 0.41 |
| 5:AD:483:GLN:O | 5:AD:485:LYS:HG2 | 2.19 | 0.41 |
| 5:AE:137:TYR:HD1 | 5:AE:143:TRP:HE1 | 1.61 | 0.41 |
| 5:AC:196:ARG:O | 5:AE:197:GLY:HA2 | 2.20 | 0.41 |
| 5:AE:326:MET:HE3 | 5:AE:326:MET:HB2 | 1.84 | 0.41 |
| 5:AE:497:PRO:HG2 | 5:AE:498:ASN:HD22 | 1.86 | 0.41 |
| 6:AF:88:TRP:HB3 | 6:AF:90:PHE:CE1 | 2.55 | 0.41 |
| 5:AD:340:VAL:HG22 | 6:AH:173:THR:HA | 2.02 | 0.41 |
| 7:AI:127:ASN:O | 7:AI:131:THR:HG23 | 2.20 | 0.41 |
| 7:AI:228:ILE:HG21 | 7:AI:244:ALA:HB2 | 2.01 | 0.41 |
| 7:AI:20:PRO:CG | 7:AI:29:ILE:HG13 | 2.49 | 0.41 |
| 7:AI:402:GLY:O | 7:BA:397:GLY:N | 2.47 | 0.41 |
| 7:AJ:248:ALA:O | 7:AJ:252:GLY:N | 2.47 | 0.41 |
| 1:B:148:ARG:HG2 | 1:B:149:GLU:HG3 | 2.01 | 0.41 |
| 1:B:299:ASN:OD1 | 1:B:300:ILE:N | 2.52 | 0.41 |
| 1:B:322:ILE:HG13 | 1:B:323:GLU:N | 2.35 | 0.41 |
| 7:AI:447:HIS:CE1 | 7:BA:445:HIS:CE1 | 3.07 | 0.41 |
| 7:BA:77:THR:OG1 | 7:BA:78:PRO:HD2 | 2.20 | 0.41 |
| 10:BE:312:GLY:HA2 | 10:BE:313:PRO:HA | 1.80 | 0.41 |
| 1:BI:62:TYR:CZ | 1:BI:66:TYR:HE2 | 2.38 | 0.41 |
| 2:BJ:224:LEU:HD23 | 2:BJ:224:LEU:O | 2.21 | 0.41 |
| 2:BJ:251:ASP:OD2 | 2:BJ:252:LYS:HG3 | 2.20 | 0.41 |
| 2:BJ:9:THR:OG1 | 2:BJ:10:SER:N | 2.51 | 0.41 |
| 2:C:151:PHE:HB3 | 2:C:166:PHE:CZ | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:CA:140:GLY:HA2 | 3:CA:163:SER:OG | 2.19 | 0.41 |
| 3:CB:134:LEU:HD23 | 3:CB:134:LEU:HA | 1.72 | 0.41 |
| 4:CC:251:ASN:N | 4:CC:266:SER:O | 2.53 | 0.41 |
| 4:CC:43:GLY:HA2 | 4:CC:62:HIS:CE1 | 2.55 | 0.41 |
| 4:CD:22:ASP:O | 4:CD:26:ASP:N | 2.26 | 0.41 |
| 5:CF:318:GLN:HB3 | 6:DA:4:LEU:HD12 | 2.02 | 0.41 |
| 5:CF:89:TYR:HB3 | 5:CG:98:VAL:HG13 | 2.02 | 0.41 |
| 5:CG:262:GLN:HA | 5:CG:381:ILE:O | 2.20 | 0.41 |
| 5:CH:118:LYS:HA | 5:CH:142:ARG:CZ | 2.51 | 0.41 |
| 5:CH:213:GLY:HA2 | 5:CH:221:GLU:HB2 | 2.02 | 0.41 |
| 5:CH:371:PHE:HZ | 5:CH:373:SER:HB3 | 1.84 | 0.41 |
| 6:CJ:195:LEU:HA | 6:CJ:215:PHE:HD1 | 1.85 | 0.41 |
| 7:DB:146:SER:N | 7:DB:149:GLN:HB2 | 2.35 | 0.41 |
| 7:DB:43:GLY:HA3 | 7:DC:39:ILE:HG23 | 2.02 | 0.41 |
| 7:DB:300:LEU:HB3 | 7:DC:302:ILE:HD13 | 2.02 | 0.41 |
| 7:DC:515:TRP:CZ3 | 7:DD:439:ILE:HG12 | 2.56 | 0.41 |
| 7:DD:405:ARG:HB2 | 7:DD:430:THR:OG1 | 2.20 | 0.41 |
| 10:DH:322:ASP:O | 10:DH:342:PHE:HB2 | 2.19 | 0.41 |
| 12:DJ:185:VAL:HG23 | 12:DJ:186:THR:N | 2.35 | 0.41 |
| 1:EA:222:THR:C | 1:EA:223:ILE:HG12 | 2.40 | 0.41 |
| 1:EA:243:ILE:HG21 | 1:EA:243:ILE:HD13 | 1.90 | 0.41 |
| 1:EA:472:ASP:O | 1:EA:473:HIS:CG | 2.73 | 0.41 |
| 1:EB:209:TRP:O | 1:EB:210:THR:C | 2.58 | 0.41 |
| 1:EB:257:ILE:HG22 | 1:EB:258:GLY:N | 2.36 | 0.41 |
| 2:EC:300:LEU:N | 2:EC:301:PRO:CD | 2.84 | 0.41 |
| 2:EC:306:ARG:C | 2:EC:307:ILE:HD12 | 2.41 | 0.41 |
| 2:EC:146:LEU:HA | 2:EC:585:MET:HA | 2.02 | 0.41 |
| 2:EC:21:VAL:HG23 | 2:EC:69:PHE:HB3 | 2.02 | 0.41 |
| 2:EC:752:TYR:O | 2:EC:753:ASN:OD1 | 2.39 | 0.41 |
| 3:ED:194:ILE:HG12 | 3:ED:223:TRP:HZ3 | 1.84 | 0.41 |
| 3:ED:45:GLU:HA | 3:ED:46:PRO:HD3 | 1.95 | 0.41 |
| 3:EE:254:ASP:CG | 3:EE:256:VAL:HG12 | 2.40 | 0.41 |
| 3:ED:316:PRO:HG2 | 3:EE:6:VAL:HG13 | 2.02 | 0.41 |
| 4:EG:124:ILE:HB | 4:EG:137:LEU:HB3 | 2.01 | 0.41 |
| 4:EH:17:ASN:OD1 | 4:EH:18:ALA:N | 2.53 | 0.41 |
| 5:EI:264:ARG:NH2 | 6:FC:3:LEU:HD13 | 2.34 | 0.41 |
| 5:EI:258:TYR:CE1 | 5:EI:384:THR:HG23 | 2.55 | 0.41 |
| 5:EJ:169:VAL:HG13 | 5:EJ:174:GLN:OE1 | 2.20 | 0.41 |
| 5:FA:338:ASP:HB3 | 5:FA:349:TRP:HD1 | 1.78 | 0.41 |
| 5:FA:303:PRO:HD2 | 5:FA:365:ILE:HD13 | 2.02 | 0.41 |
| 5:FA:497:PRO:HG2 | 5:FA:498:ASN:ND2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:FA:89:TYR:HA | 5:FA:137:TYR:CD2 | 2.55 | 0.41 |
| 6:FC:117:THR:H | 6:FC:120:MET:HE3 | 1.84 | 0.41 |
| 6:FC:195:LEU:HA | 6:FC:215:PHE:HD1 | 1.85 | 0.41 |
| 6:FC:88:TRP:HB3 | 6:FC:90:PHE:CE1 | 2.55 | 0.41 |
| 7:FE:19:ASP:HB3 | 7:FG:33:GLN:OE1 | 2.20 | 0.41 |
| 7:FE:246:THR:HG1 | 7:FE:249:THR:H | 1.61 | 0.41 |
| 7:FE:255:SER:N | 7:FE:278:SER:OG | 2.53 | 0.41 |
| 7:FE:429:CYS:HA | 7:FG:511:GLU:OE1 | 2.19 | 0.41 |
| 7:FE:77:THR:CG2 | 7:FE:80:THR:H | 2.33 | 0.41 |
| 7:FF:183:ALA:HB2 | 7:FF:189:GLY:O | 2.20 | 0.41 |
| 7:FF:451:PHE:HD1 | 7:FF:469:VAL:HG13 | 1.85 | 0.41 |
| 7:FG:232:THR:HG23 | 7:FG:235:GLU:H | 1.85 | 0.41 |
| 7:FG:417:ASN:O | 7:FG:424:ARG:NH1 | 2.53 | 0.41 |
| 8:FI:89:GLN:HB3 | 8:FI:134:PRO:CG | 2.50 | 0.41 |
| 9:FJ:36:LEU:HD23 | 9:FJ:36:LEU:HA | 1.89 | 0.41 |
| 4:G:17:ASN:OD1 | 4:G:18:ALA:N | 2.53 | 0.41 |
| 11:GB:43:TYR:CE2 | 11:GB:180:PHE:HB2 | 2.49 | 0.41 |
| 12:GC:187:GLY:C | 12:GC:188:LEU:HD12 | 2.41 | 0.41 |
| 12:DJ:215:MET:HE1 | 12:GC:99:SER:HB2 | 2.01 | 0.41 |
| 1:GD:111:MET:O | 1:GD:111:MET:HG3 | 2.20 | 0.41 |
| 1:GD:105:ALA:HB2 | 1:GD:275:THR:HG21 | 2.02 | 0.41 |
| 1:GD:572:TYR:CE2 | 1:GD:574:GLY:HA3 | 2.56 | 0.41 |
| 1:GE:229:THR:OG1 | 1:GE:233:ASN:OD1 | 2.34 | 0.41 |
| 1:GE:174:ARG:HA | 1:GE:270:ILE:O | 2.19 | 0.41 |
| 1:GE:299:ASN:OD1 | 1:GE:300:ILE:N | 2.52 | 0.41 |
| 1:GE:485:VAL:HG22 | 1:GE:624:TYR:CD1 | 2.55 | 0.41 |
| 2:GF:146:LEU:C | 2:GF:146:LEU:HD12 | 2.39 | 0.41 |
| 2:GF:457:ASN:O | 2:GF:458:ASP:C | 2.58 | 0.41 |
| 2:GF:750:VAL:HG23 | 2:GF:751:LEU:H | 1.84 | 0.41 |
| 2:GF:752:TYR:O | 2:GF:753:ASN:OD1 | 2.39 | 0.41 |
| 3:GG:255:SER:O | 3:GG:258:PHE:N | 2.53 | 0.41 |
| 4:H:17:ASN:OD1 | 4:H:18:ALA:N | 2.53 | 0.41 |
| 5:HB:118:LYS:HA | 5:HB:142:ARG:NH2 | 2.35 | 0.41 |
| 5:HB:222:LEU:HD11 | 5:HB:224:PRO:HD2 | 2.01 | 0.41 |
| 5:HB:336:SER:HB3 | 5:HB:348:THR:O | 2.20 | 0.41 |
| 5:HB:36:GLU:OE1 | 5:HB:66:LYS:HG2 | 2.19 | 0.41 |
| 5:HC:569:TYR:CD1 | 5:HD:544:VAL:HA | 2.54 | 0.41 |
| 5:HD:186:TYR:O | 5:HD:227:GLY:HA3 | 2.20 | 0.41 |
| 6:HF:195:LEU:HA | 6:HF:215:PHE:HD1 | 1.85 | 0.41 |
| 6:HG:88:TRP:HB3 | 6:HG:90:PHE:CE1 | 2.55 | 0.41 |
| 7:HH:363:HIS:CD2 | 7:HH:396:ARG:HD3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:466:SER:HB3 | 7:HH:468:PHE:CE2 | 2.54 | 0.41 |
| 7:HH:451:PHE:CE1 | 7:HH:470:GLY:HA2 | 2.56 | 0.41 |
| 7:HI:77:THR:HG21 | 7:HJ:72:ASN:CG | 2.41 | 0.41 |
| 7:HJ:232:THR:HG23 | 7:HJ:235:GLU:H | 1.85 | 0.41 |
| 7:HJ:20:PRO:CB | 7:HJ:29:ILE:HG13 | 2.48 | 0.41 |
| 5:I:18:TYR:CE1 | 5:I:20:ARG:HB3 | 2.55 | 0.41 |
| 5:I:336:SER:HB3 | 5:I:348:THR:O | 2.20 | 0.41 |
| 5:I:261:ARG:HB2 | 5:I:383:ILE:HB | 2.01 | 0.41 |
| 12:IF:187:GLY:C | 12:IF:188:LEU:HD12 | 2.41 | 0.41 |
| 5:J:255:ARG:HH21 | 5:K:249:ASP:HB2 | 1.85 | 0.41 |
| 5:J:262:GLN:HA | 5:J:381:ILE:O | 2.20 | 0.41 |
| 5:J:275:SER:OG | 5:J:281:TYR:HA | 2.18 | 0.41 |
| 5:J:430:TRP:HA | 5:J:431:PRO:C | 2.40 | 0.41 |
| 5:J:38:GLY:HA2 | 5:J:43:PRO:HA | 2.02 | 0.41 |
| 5:J:48:ALA:C | 5:J:49:TRP:CD1 | 2.93 | 0.41 |
| 5:K:454:TYR:O | 5:K:600:ARG:NH1 | 2.43 | 0.41 |
| 5:K:89:TYR:HA | 5:K:137:TYR:CD2 | 2.55 | 0.41 |
| 6:M:64:ILE:HG23 | 6:M:217:ARG:HH12 | 1.84 | 0.41 |
| 7:O:139:ASN:N | 7:Q:143:LYS:HG2 | 2.35 | 0.41 |
| 7:O:197:ALA:O | 7:O:201:GLN:HG3 | 2.20 | 0.41 |
| 7:O:497:ASN:OD1 | 7:O:500:TYR:N | 2.53 | 0.41 |
| 7:O:99:ARG:N | 7:P:95:TYR:HD1 | 2.18 | 0.41 |
| 7:Q:417:ASN:O | 7:Q:424:ARG:NH1 | 2.54 | 0.41 |
| 7:Q:475:LEU:HD23 | 7:Q:475:LEU:HA | 1.84 | 0.41 |
| 11:V:177:ILE:HG23 | 11:V:178:ASN:N | 2.35 | 0.41 |
| 12:W:15:ASP:O | 12:W:16:PHE:CD1 | 2.73 | 0.41 |
| 12:W:124:MET:HG3 | 12:W:170:ASN:ND2 | 2.35 | 0.41 |
| 12:W:230:TYR:CE1 | 12:IF:22:PHE:CZ | 3.08 | 0.41 |
| 1:X:55:VAL:O | 1:X:58:ASP:HB3 | 2.20 | 0.41 |
| 1:Y:158:ASN:CG | 1:Y:160:GLN:HG2 | 2.40 | 0.41 |
| 13:YA:293[B]:ASN:HA | 13:YA:296[B]:LEU:HB2 | 2.01 | 0.41 |
| 13:YA:38[D]:GLN:O | 13:YA:46[D]:GLY:HA2 | 2.20 | 0.41 |
| 13:YA:389[B]:TYR:O | 13:YA:405[B]:ASP:HB2 | 2.19 | 0.41 |
| 13:YA:454[D]:LYS:C | 13:YA:455[D]:LYS:HG3 | 2.39 | 0.41 |
| 13:YA:553[E]:LYS:HA | 13:YC:560[E]:ILE:O | 2.21 | 0.41 |
| 13:YA:83[D]:TYR:OH | 13:YA:85[D]:HIS:HE1 | 2.03 | 0.41 |
| 13:YB:154[F]:THR:H | 13:YB:182[F]:ARG:NH2 | 2.17 | 0.41 |
| 13:YB:187[F]:ARG:HA | 13:YB:187[F]:ARG:HD3 | 1.86 | 0.41 |
| 13:YB:373[B]:ARG:NE | 13:YB:373[B]:ARG:HA | 2.31 | 0.41 |
| 13:YB:418[E]:THR:HG21 | 13:YC:428[E]:GLY:CA | 2.49 | 0.41 |
| 13:YB:410[F]:GLU:O | 13:YB:426[F]:PRO:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:439[C]:TYR:HB3 | 13:YB:441[C]:ILE:CD1 | 2.49 | 0.41 |
| 13:YB:38[C]:GLN:O | 13:YB:46[C]:GLY:HA2 | 2.20 | 0.41 |
| 13:YC:187[F]:ARG:HA | 13:YC:187[F]:ARG:HD3 | 1.86 | 0.41 |
| 13:YC:195[B]:GLU:HG2 | 13:YC:197[B]:TYR:CE2 | 2.54 | 0.41 |
| 13:YC:209[E]:GLN:HB3 | 13:YC:211[E]:VAL:HG23 | 2.03 | 0.41 |
| 13:YC:277[F]:LEU:HD23 | 13:YC:277[F]:LEU:HA | 1.80 | 0.41 |
| 13:YC:293[E]:ASN:HA | 13:YC:296[E]:LEU:HB2 | 2.01 | 0.41 |
| 13:YC:439[F]:TYR:HB3 | 13:YC:441[F]:ILE:CD1 | 2.49 | 0.41 |
| 13:YC:454[D]:LYS:C | 13:YC:455[D]:LYS:HG3 | 2.39 | 0.41 |
| 13:YB:476[D]:GLY:HA3 | 13:YC:469[D]:ASN:HA | 2.00 | 0.41 |
| 13:YC:66[E]:MET:HA | 13:YC:66[E]:MET:HE3 | 2.01 | 0.41 |
| 13:YC:83[D]:TYR:OH | 13:YC:85[D]:HIS:HE1 | 2.03 | 0.41 |
| 10:ID:286:VAL:HG13 | 14:YD:100[B]:LYS:CE | 2.50 | 0.41 |
| 14:YD:112[F]:ILE:HB | 14:YD:140[F]:TYR:OH | 2.19 | 0.41 |
| 14:YD:124[B]:PHE:CZ | 14:YD:135[B]:MET:HG2 | 2.55 | 0.41 |
| 14:YD:172[B]:TYR:CZ | 14:YD:176[B]:VAL:HG21 | 2.54 | 0.41 |
| 14:YD:43[A]:SER:O | 14:YD:189[A]:TRP:HB2 | 2.20 | 0.41 |
| 14:YD:43[C]:SER:O | 14:YD:189[C]:TRP:HB2 | 2.20 | 0.41 |
| 14:YD:47[D]:ARG:NH1 | 14:YD:341[D]:GLU:OE1 | 2.53 | 0.41 |
| 14:YD:345[D]:GLU:HB3 | 14:YD:352[D]:VAL:HG13 | 2.02 | 0.41 |
| 14:YD:43[F]:SER:O | 14:YD:189[F]:TRP:HB2 | 2.20 | 0.41 |
| 14:YE:124[E]:PHE:CZ | 14:YE:135[E]:MET:HG2 | 2.55 | 0.41 |
| 13:YC:100[E]:TYR:CD2 | 14:YE:258[E]:PHE:HD1 | 2.38 | 0.41 |
| 14:YE:290[D]:ASN:C | 14:YE:290[D]:ASN:OD1 | 2.58 | 0.41 |
| 14:YE:238[A]:THR:N | 14:YE:307[A]:TYR:O | 2.53 | 0.41 |
| 14:YE:238[C]:THR:N | 14:YE:307[C]:TYR:O | 2.52 | 0.41 |
| 14:YE:364[A]:LEU:HD22 | 14:YE:364[A]:LEU:HA | 1.79 | 0.41 |
| 14:YE:45[A]:TYR:HD1 | 14:YE:45[A]:TYR:HA | 1.68 | 0.41 |
| 14:YE:75[E]:ALA:HB2 | 14:YE:83[E]:VAL:HA | 2.01 | 0.41 |
| 14:YF:124[E]:PHE:CZ | 14:YF:135[E]:MET:HG2 | 2.55 | 0.41 |
| 14:YF:172[E]:TYR:CZ | 14:YF:176[E]:VAL:HG21 | 2.54 | 0.41 |
| 14:YF:174[A]:ARG:CG | 14:YF:188[A]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:174[F]:ARG:CG | 14:YF:188[F]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:259[C]:LEU:HA | 14:YF:259[C]:LEU:HD23 | 1.82 | 0.41 |
| 2:Z:347:GLU:N | 2:Z:347:GLU:OE1 | 2.42 | 0.41 |
| 2:Z:644:ASP:HB2 | 2:Z:646:ARG:HG2 | 2.01 | 0.41 |
| 2:Z:73:ASP:HB3 | 2:Z:76:THR:HG21 | 2.02 | 0.41 |
| 15:ZA:26[F]:GLN:NE2 | 15:ZA:29[F]:VAL:H | 1.92 | 0.41 |
| 1:A:360:VAL:HG23 | 1:A:375:ALA:O | 2.20 | 0.41 |
| 1:A:377:LYS:HD3 | 1:A:641:VAL:HG21 | 2.02 | 0.41 |
| 5:AC:118:LYS:HA | 5:AC:142:ARG:NH2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:137:TYR:HA | 5:AC:143:TRP:HD1 | 1.84 | 0.41 |
| 5:AC:18:TYR:CE1 | 5:AC:20:ARG:HB3 | 2.55 | 0.41 |
| 5:AC:202:TYR:CD1 | 5:AC:225:LEU:HD12 | 2.54 | 0.41 |
| 5:AD:38:GLY:HA2 | 5:AD:43:PRO:HA | 2.02 | 0.41 |
| 5:AD:395:THR:OG1 | 5:AD:396:LYS:N | 2.52 | 0.41 |
| 5:AC:590:GLN:O | 5:AD:521:GLY:HA3 | 2.20 | 0.41 |
| 5:AE:151:ILE:HG23 | 5:AE:152:ASP:N | 2.34 | 0.41 |
| 5:AE:213:GLY:HA2 | 5:AE:221:GLU:HB2 | 2.02 | 0.41 |
| 5:AE:181:PHE:HE2 | 5:AE:246:THR:HG22 | 1.84 | 0.41 |
| 6:AF:199:GLN:HB2 | 6:AG:203:LEU:CD2 | 2.49 | 0.41 |
| 6:AF:13:ARG:NH1 | 6:AH:47:PHE:CZ | 2.88 | 0.41 |
| 7:AI:146:SER:N | 7:AI:149:GLN:HB2 | 2.35 | 0.41 |
| 7:AJ:183:ALA:HB2 | 7:AJ:189:GLY:O | 2.20 | 0.41 |
| 7:AI:60:ILE:HG22 | 7:AJ:51:SER:C | 2.40 | 0.41 |
| 7:AI:78:PRO:HB2 | 7:AJ:69:GLY:HA2 | 2.01 | 0.41 |
| 7:AI:99:ARG:N | 7:AJ:95:TYR:HD1 | 2.18 | 0.41 |
| 1:B:190:LYS:O | 1:B:191:ASN:HB2 | 2.20 | 0.41 |
| 1:B:307:ASP:N | 1:B:307:ASP:OD1 | 2.53 | 0.41 |
| 1:B:524:VAL:HG13 | 1:B:529:GLY:O | 2.19 | 0.41 |
| 1:B:60:LEU:HA | 1:B:60:LEU:HD23 | 1.73 | 0.41 |
| 1:B:611:LEU:HD11 | 1:B:616:PHE:CE2 | 2.54 | 0.41 |
| 7:BA:232:THR:CG2 | 7:BA:235:GLU:H | 2.34 | 0.41 |
| 7:BA:405:ARG:HB2 | 7:BA:430:THR:OG1 | 2.20 | 0.41 |
| 10:BE:62:LEU:O | 10:BE:128:LEU:HD12 | 2.20 | 0.41 |
| 10:BE:286:VAL:HG13 | 14:YF:100[A]:LYS:HE2 | 2.02 | 0.41 |
| 12:BG:185:VAL:HG23 | 12:BG:186:THR:N | 2.35 | 0.41 |
| 1:BH:205:GLU:O | 1:BH:206:TRP:HD1 | 2.04 | 0.41 |
| 1:BH:175:THR:O | 1:BH:270:ILE:HG22 | 2.20 | 0.41 |
| 1:BH:23:GLY:HA2 | 1:BH:68:GLN:NE2 | 2.35 | 0.41 |
| 1:BI:190:LYS:O | 1:BI:191:ASN:HB2 | 2.20 | 0.41 |
| 1:BI:341:THR:OG1 | 1:BI:342:ALA:N | 2.51 | 0.41 |
| 1:BI:530:LEU:HD12 | 1:BI:532:GLU:H | 1.84 | 0.41 |
| 1:BI:619:GLN:H | 1:BI:619:GLN:CD | 2.21 | 0.41 |
| 1:BH:227:ARG:HH21 | 1:BI:81:ARG:NH2 | 2.18 | 0.41 |
| 2:BJ:131:ASN:OD1 | 2:BJ:133:ASP:N | 2.50 | 0.41 |
| 2:BJ:906:LEU:HD12 | 2:BJ:907:LYS:N | 2.35 | 0.41 |
| 2:C:431:TYR:HB3 | 2:C:485:TYR:OH | 2.20 | 0.41 |
| 2:C:579:LYS:HB3 | 2:C:579:LYS:HE3 | 1.86 | 0.41 |
| 2:C:701:TRP:O | 2:C:701:TRP:CG | 2.72 | 0.41 |
| 1:B:213:SER:HA | 2:C:733:ASP:CG | 2.40 | 0.41 |
| 4:CC:17:ASN:OD1 | 4:CC:18:ALA:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:CC:22:ASP:O | 4:CC:26:ASP:N | 2.26 | 0.41 |
| 4:CD:44:ASP:O | 4:CD:59:GLN:NE2 | 2.52 | 0.41 |
| 4:CD:216:THR:CG2 | 4:CE:222:LEU:HD13 | 2.51 | 0.41 |
| 5:CF:137:TYR:HA | 5:CF:143:TRP:CD1 | 2.55 | 0.41 |
| 5:CF:239:GLY:O | 7:DB:5:THR:N | 2.46 | 0.41 |
| 5:CG:137:TYR:HB2 | 5:CG:143:TRP:HE1 | 1.86 | 0.41 |
| 5:CG:38:GLY:HA2 | 5:CG:43:PRO:HA | 2.02 | 0.41 |
| 5:CG:454:TYR:HD1 | 5:CG:458:THR:HG21 | 1.85 | 0.41 |
| 5:CG:460:TYR:CE1 | 5:CH:458:THR:HG23 | 2.55 | 0.41 |
| 5:CG:147:LYS:HG2 | 5:CH:154:ILE:O | 2.20 | 0.41 |
| 5:CH:192:ARG:HB2 | 5:CH:245:GLU:H | 1.85 | 0.41 |
| 5:CH:288:MET:CE | 5:CH:292:PRO:HD3 | 2.50 | 0.41 |
| 5:CG:443:PHE:O | 5:CH:408:VAL:HG13 | 2.20 | 0.41 |
| 3:D:138:ASP:HA | 3:D:150:LYS:HE3 | 2.03 | 0.41 |
| 3:D:95:TRP:CZ2 | 3:D:169:PRO:HD3 | 2.55 | 0.41 |
| 3:D:191:LEU:HD23 | 3:D:191:LEU:HA | 1.82 | 0.41 |
| 5:CG:339:GLU:HG2 | 6:DA:173:THR:HB | 2.02 | 0.41 |
| 7:DB:102:THR:O | 7:DB:105:GLU:N | 2.52 | 0.41 |
| 7:DB:232:THR:HG23 | 7:DB:235:GLU:H | 1.85 | 0.41 |
| 7:DB:49:ASP:OD1 | 7:DB:50:ALA:N | 2.54 | 0.41 |
| 7:DB:77:THR:CG2 | 7:DB:80:THR:H | 2.33 | 0.41 |
| 7:DC:255:SER:HB2 | 7:DC:261:GLY:O | 2.20 | 0.41 |
| 7:DC:343:VAL:HG13 | 7:DC:524:LYS:O | 2.20 | 0.41 |
| 7:DD:166:GLN:O | 7:DD:170:ILE:HB | 2.20 | 0.41 |
| 7:DD:20:PRO:CB | 7:DD:29:ILE:HG13 | 2.48 | 0.41 |
| 7:DD:232:THR:CG2 | 7:DD:235:GLU:H | 2.34 | 0.41 |
| 7:DC:262:VAL:CG2 | 7:DD:260:ARG:HB3 | 2.51 | 0.41 |
| 7:DB:346:ILE:O | 7:DD:348:MET:HB2 | 2.20 | 0.41 |
| 7:DC:516:ASN:OD1 | 7:DD:438:GLN:HB2 | 2.20 | 0.41 |
| 7:DC:476:ASP:OD2 | 7:DD:454:HIS:HE1 | 2.02 | 0.41 |
| 7:DC:75:ALA:HB1 | 7:DD:75:ALA:HB1 | 2.02 | 0.41 |
| 7:DB:76:VAL:N | 7:DD:76:VAL:O | 2.33 | 0.41 |
| 10:DH:221:ALA:O | 10:DH:225:ILE:N | 2.46 | 0.41 |
| 11:DI:71:TRP:O | 11:DI:74:LEU:N | 2.53 | 0.41 |
| 3:E:268:GLY:HA3 | 3:E:318:ILE:O | 2.20 | 0.41 |
| 1:EA:146:VAL:HG11 | 1:EA:172:ILE:HG12 | 2.01 | 0.41 |
| 1:EA:205:GLU:O | 1:EA:206:TRP:HD1 | 2.04 | 0.41 |
| 1:EA:414:LEU:HD23 | 1:EA:486:ARG:HE | 1.84 | 0.41 |
| 1:EB:144:ASN:N | 1:EB:144:ASN:OD1 | 2.47 | 0.41 |
| 1:EB:190:LYS:O | 1:EB:191:ASN:HB2 | 2.20 | 0.41 |
| 1:EB:299:ASN:OD1 | 1:EB:300:ILE:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EB:56:LEU:HA | 2:EC:653:MET:HE1 | 2.01 | 0.41 |
| 2:EC:151:PHE:HB3 | 2:EC:166:PHE:CZ | 2.55 | 0.41 |
| 2:EC:246:TYR:HE1 | 2:EC:255:TYR:CD1 | 2.35 | 0.41 |
| 2:EC:338:PHE:CE2 | 2:EC:342:SER:O | 2.69 | 0.41 |
| 2:EC:664:PHE:HB2 | 9:FJ:15:MET:CB | 2.50 | 0.41 |
| 2:EC:729:SER:OG | 2:EC:730:ARG:N | 2.54 | 0.41 |
| 2:EC:897:THR:O | 2:EC:898:MET:HE2 | 2.19 | 0.41 |
| 2:EC:976:SER:C | 2:EC:977:ILE:HG13 | 2.40 | 0.41 |
| 3:ED:114:CYS:HA | 3:ED:120:ASN:HD21 | 1.85 | 0.41 |
| 3:EE:150:LYS:HG3 | 3:EE:160:TRP:CG | 2.55 | 0.41 |
| 3:EE:268:GLY:HA3 | 3:EE:318:ILE:O | 2.20 | 0.41 |
| 3:EE:80:LYS:HG2 | 3:EE:81:VAL:H | 1.85 | 0.41 |
| 4:EF:43:GLY:HA2 | 4:EF:62:HIS:CE1 | 2.55 | 0.41 |
| 4:EG:192:PHE:O | 4:EG:261:VAL:N | 2.51 | 0.41 |
| 4:EG:213:LYS:HE3 | 4:EG:249:ILE:HG12 | 2.03 | 0.41 |
| 4:EG:251:ASN:N | 4:EG:266:SER:O | 2.53 | 0.41 |
| 4:EH:251:ASN:N | 4:EH:266:SER:O | 2.53 | 0.41 |
| 5:EI:107:VAL:HB | 5:EI:126:ILE:HB | 2.01 | 0.41 |
| 5:EJ:153:LYS:HG2 | 5:EJ:154:ILE:N | 2.32 | 0.41 |
| 4:F:131:LYS:HD3 | 4:F:161:ASN:HD22 | 1.85 | 0.41 |
| 5:FA:181:PHE:HE2 | 5:FA:246:THR:HG22 | 1.85 | 0.41 |
| 5:FA:304:ILE:HG21 | 5:FA:309:LEU:HG | 2.02 | 0.41 |
| 5:EJ:569:TYR:CE1 | 5:FA:544:VAL:HG22 | 2.55 | 0.41 |
| 6:FB:109:VAL:HG13 | 6:FB:178:ILE:HG21 | 2.02 | 0.41 |
| 6:FD:109:VAL:HG13 | 6:FD:178:ILE:HG21 | 2.02 | 0.41 |
| 7:FE:232:THR:HG23 | 7:FE:235:GLU:H | 1.86 | 0.41 |
| 7:FF:232:THR:O | 7:FF:236:VAL:HG22 | 2.20 | 0.41 |
| 7:FG:232:THR:CG2 | 7:FG:235:GLU:H | 2.34 | 0.41 |
| 7:FE:501:THR:HB | 7:FG:422:LYS:NZ | 2.35 | 0.41 |
| 7:FG:489:GLU:OE2 | 7:FG:502:LEU:N | 2.53 | 0.41 |
| 7:FG:489:GLU:CD | 7:FG:502:LEU:H | 2.22 | 0.41 |
| 1:GD:132:LEU:HD23 | 1:GD:132:LEU:HA | 1.77 | 0.41 |
| 1:GD:251:ALA:CB | 1:GE:337:GLN:HG2 | 2.50 | 0.41 |
| 1:GD:175:THR:O | 1:GD:270:ILE:HG22 | 2.20 | 0.41 |
| 1:GD:384:LEU:HD23 | 1:GD:384:LEU:HA | 1.83 | 0.41 |
| 1:GD:390:GLU:O | 1:GD:394:ASN:ND2 | 2.53 | 0.41 |
| 1:GD:472:ASP:O | 1:GD:473:HIS:CG | 2.73 | 0.41 |
| 1:GE:530:LEU:HD12 | 1:GE:532:GLU:H | 1.84 | 0.41 |
| 2:GF:251:ASP:OD2 | 2:GF:252:LYS:HG3 | 2.20 | 0.41 |
| 2:GF:729:SER:OG | 2:GF:730:ARG:N | 2.54 | 0.41 |
| 1:GE:213:SER:HA | 2:GF:733:ASP:CG | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:GF:906:LEU:HD12 | 2:GF:907:LYS:N | 2.35 | 0.41 |
| 2:GF:976:SER:C | 2:GF:977:ILE:HG13 | 2.40 | 0.41 |
| 3:GG:254:ASP:HB3 | 3:GG:257:TYR:CD2 | 2.54 | 0.41 |
| 4:GI:172:GLU:HA | 4:GJ:166:SER:N | 2.35 | 0.41 |
| 4:GJ:107:VAL:O | 4:GJ:148:LEU:N | 2.39 | 0.41 |
| 4:GJ:224:ASP:OD2 | 4:GJ:227:ASN:HB2 | 2.19 | 0.41 |
| 4:H:224:ASP:OD2 | 4:H:227:ASN:HB2 | 2.19 | 0.41 |
| 5:HB:103:ASN:CG | 5:HB:104:VAL:H | 2.24 | 0.41 |
| 5:HB:137:TYR:HA | 5:HB:143:TRP:CD1 | 2.55 | 0.41 |
| 5:HB:542:LEU:HD21 | 5:HC:569:TYR:CZ | 2.55 | 0.41 |
| 5:HC:290:SER:CA | 5:HC:371:PHE:H | 2.33 | 0.41 |
| 5:HC:38:GLY:HA2 | 5:HC:43:PRO:HA | 2.03 | 0.41 |
| 5:HC:480:LEU:HA | 5:HC:480:LEU:HD23 | 1.81 | 0.41 |
| 5:HC:567:THR:O | 5:HD:551:ILE:HA | 2.19 | 0.41 |
| 6:HF:42:GLN:OE1 | 6:HF:42:GLN:N | 2.52 | 0.41 |
| 6:HG:90:PHE:CD2 | 6:HG:126:VAL:HG22 | 2.45 | 0.41 |
| 6:HG:145:SER:O | 6:HG:159:THR:N | 2.45 | 0.41 |
| 5:HB:316:ILE:HD13 | 6:HG:7:LYS:HG3 | 2.03 | 0.41 |
| 7:HH:171:LYS:HA | 7:HH:174:ALA:HB3 | 2.03 | 0.41 |
| 7:HH:44:VAL:HG21 | 7:HI:25:PHE:HB3 | 2.03 | 0.41 |
| 7:HH:501:THR:HB | 7:HJ:422:LYS:NZ | 2.35 | 0.41 |
| 7:HH:503:ASN:ND2 | 7:HJ:445:HIS:HB2 | 2.35 | 0.41 |
| 5:I:321:ALA:HA | 5:I:358:VAL:CB | 2.44 | 0.41 |
| 5:J:117:ILE:HG13 | 5:J:118:LYS:H | 1.85 | 0.41 |
| 5:J:186:TYR:HB3 | 5:J:227:GLY:O | 2.20 | 0.41 |
| 5:J:49:TRP:HH2 | 5:J:96:ARG:HE | 1.67 | 0.41 |
| 5:K:133:LEU:HA | 5:K:133:LEU:HD23 | 1.81 | 0.41 |
| 5:J:147:LYS:HG2 | 5:K:154:ILE:O | 2.20 | 0.41 |
| 5:K:304:ILE:O | 5:K:304:ILE:HD12 | 2.20 | 0.41 |
| 5:I:30:PHE:CE1 | 5:K:30:PHE:CE1 | 3.05 | 0.41 |
| 6:L:90:PHE:O | 6:L:154:SER:HB2 | 2.19 | 0.41 |
| 7:O:190:VAL:HG23 | 7:P:188:GLN:HB3 | 2.01 | 0.41 |
| 7:P:255:SER:HB2 | 7:P:261:GLY:O | 2.20 | 0.41 |
| 8:S:88:TRP:CE3 | 8:S:134:PRO:HD3 | 2.53 | 0.41 |
| 8:S:91:ILE:HG22 | 8:S:107:TYR:HB3 | 2.02 | 0.41 |
| 12:W:191:LEU:HA | 12:W:191:LEU:HD23 | 1.82 | 0.41 |
| 1:X:167:LEU:HD23 | 1:X:167:LEU:HA | 1.76 | 0.41 |
| 1:X:275:THR:O | 1:X:275:THR:OG1 | 2.36 | 0.41 |
| 1:X:609:ILE:HG22 | 1:X:611:LEU:HG | 2.01 | 0.41 |
| 1:Y:257:ILE:HG22 | 1:Y:258:GLY:N | 2.36 | 0.41 |
| 1:Y:270:ILE:HD13 | 1:Y:270:ILE:HG21 | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:342:ALA:C | 1:Y:344:ASP:N | 2.74 | 0.41 |
| 1:Y:62:TYR:CZ | 1:Y:66:TYR:HE2 | 2.38 | 0.41 |
| 13:YA:195[F]:GLU:HG2 | 13:YA:197[F]:TYR:CE2 | 2.54 | 0.41 |
| 13:YA:209[D]:GLN:HB3 | 13:YA:211[D]:VAL:HG23 | 2.02 | 0.41 |
| 13:YA:219[E]:LYS:HB2 | 13:YA:219[E]:LYS:HE3 | 1.80 | 0.41 |
| 13:YA:239[B]:GLU:CD | 13:YA:239[B]:GLU:H | 2.24 | 0.41 |
| 13:YA:564[A]:GLN:HG3 | 13:YA:566[A]:THR:HG22 | 2.01 | 0.41 |
| 13:YA:76[D]:PRO:HB2 | 13:YA:98[D]:GLY:CA | 2.51 | 0.41 |
| 13:YA:76[B]:PRO:HB3 | 13:YA:96[B]:VAL:O | 2.20 | 0.41 |
| 13:YB:24[E]:LEU:HD23 | 14:YE:259[E]:LEU:CD2 | 2.50 | 0.41 |
| 13:YB:293[E]:ASN:HA | 13:YB:296[E]:LEU:HB2 | 2.01 | 0.41 |
| 13:YB:336[C]:LEU:HD12 | 13:YB:336[C]:LEU:HA | 1.85 | 0.41 |
| 13:YB:418[D]:THR:HG21 | 13:YC:428[D]:GLY:CA | 2.50 | 0.41 |
| 13:YB:453[C]:ASP:O | 13:YC:445[C]:ASP:HA | 2.20 | 0.41 |
| 13:YB:38[B]:GLN:O | 13:YB:46[B]:GLY:HA2 | 2.20 | 0.41 |
| 13:YB:554[A]:MET:HE3 | 13:YB:554[A]:MET:HB3 | 1.83 | 0.41 |
| 13:YB:566[F]:THR:HG23 | 13:YC:558[F]:SER:HA | 2.01 | 0.41 |
| 13:YB:76[B]:PRO:HB3 | 13:YB:96[B]:VAL:O | 2.20 | 0.41 |
| 13:YC:38[F]:GLN:O | 13:YC:46[F]:GLY:HA2 | 2.20 | 0.41 |
| 13:YC:410[D]:GLU:O | 13:YC:426[D]:PRO:HA | 2.20 | 0.41 |
| 13:YC:399[B]:HIS:ND1 | 13:YC:417[B]:PRO:HD3 | 2.36 | 0.41 |
| 13:YB:558[C]:SER:N | 13:YC:550[C]:TRP:O | 2.47 | 0.41 |
| 13:YA:553[F]:LYS:HA | 13:YC:560[F]:ILE:O | 2.21 | 0.41 |
| 14:YD:51[B]:MET:SD | 14:YD:108[B]:GLU:HA | 2.60 | 0.41 |
| 14:YD:124[F]:PHE:CZ | 14:YD:135[F]:MET:HG2 | 2.56 | 0.41 |
| 14:YD:210[A]:PRO:HB2 | 14:YD:228[A]:TYR:CD2 | 2.55 | 0.41 |
| 14:YD:230[F]:LEU:HA | 14:YD:230[F]:LEU:HD13 | 1.84 | 0.41 |
| 14:YD:259[F]:LEU:HA | 14:YD:259[F]:LEU:HD23 | 1.83 | 0.41 |
| 14:YD:259[A]:LEU:HD23 | 14:YD:259[A]:LEU:HA | 1.82 | 0.41 |
| 14:YD:290[F]:ASN:C | 14:YD:290[F]:ASN:OD1 | 2.58 | 0.41 |
| 14:YD:75[C]:ALA:HB2 | 14:YD:83[C]:VAL:HA | 2.02 | 0.41 |
| 14:YE:51[B]:MET:SD | 14:YE:108[B]:GLU:HA | 2.61 | 0.41 |
| 14:YE:172[A]:TYR:CZ | 14:YE:176[A]:VAL:HG21 | 2.54 | 0.41 |
| 14:YE:174[B]:ARG:CG | 14:YE:188[B]:VAL:HG22 | 2.51 | 0.41 |
| 14:YE:174[C]:ARG:CG | 14:YE:188[C]:VAL:HG22 | 2.51 | 0.41 |
| 14:YE:210[E]:PRO:HB2 | 14:YE:228[E]:TYR:CD2 | 2.55 | 0.41 |
| 13:YC:81[C]:ARG:HD3 | 14:YE:261[C]:SER:HA | 2.02 | 0.41 |
| 14:YE:238[B]:THR:N | 14:YE:307[B]:TYR:O | 2.53 | 0.41 |
| 14:YE:47[E]:ARG:NH1 | 14:YE:341[E]:GLU:OE1 | 2.53 | 0.41 |
| 14:YF:290[E]:ASN:C | 14:YF:290[E]:ASN:OD1 | 2.58 | 0.41 |
| 14:YF:75[C]:ALA:HB2 | 14:YF:83[C]:VAL:HA | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:ZA:26[D]:GLN:HE21 | 15:ZA:26[D]:GLN:HB2 | 1.72 | 0.41 |
| 1:A:306:ASP:N | 1:A:306:ASP:OD1 | 2.52 | 0.41 |
| 5:AC:81:LEU:HD22 | 5:AC:143:TRP:CZ3 | 2.56 | 0.41 |
| 5:AC:321:ALA:O | 5:AC:324:VAL:HG12 | 2.19 | 0.41 |
| 5:AC:84:GLY:C | 5:AC:86:VAL:H | 2.18 | 0.41 |
| 5:AD:305:ASN:HB3 | 5:AE:255:ARG:HH12 | 1.85 | 0.41 |
| 5:AD:262:GLN:HA | 5:AD:381:ILE:O | 2.20 | 0.41 |
| 5:AD:49:TRP:CD1 | 5:AD:49:TRP:N | 2.87 | 0.41 |
| 5:AE:104:VAL:HG22 | 5:AE:105:ASN:N | 2.35 | 0.41 |
| 5:AC:544:VAL:HA | 5:AE:569:TYR:CE1 | 2.55 | 0.41 |
| 6:AG:195:LEU:HA | 6:AG:215:PHE:HD1 | 1.85 | 0.41 |
| 7:AI:232:THR:HG23 | 7:AI:235:GLU:H | 1.85 | 0.41 |
| 7:AI:453:GLU:OE2 | 7:AI:471:THR:N | 2.32 | 0.41 |
| 1:B:158:ASN:CG | 1:B:160:GLN:HG2 | 2.40 | 0.41 |
| 1:B:533:ASP:O | 1:B:535:LEU:N | 2.53 | 0.41 |
| 1:B:66:TYR:O | 1:B:69:GLN:N | 2.54 | 0.41 |
| 7:BA:110:VAL:HG12 | 7:BA:111:ASN:H | 1.84 | 0.41 |
| 7:BA:147:LEU:HB2 | 7:BA:148:PRO:HD3 | 2.02 | 0.41 |
| 11:BF:166:LEU:HD23 | 11:BF:166:LEU:HA | 1.83 | 0.41 |
| 12:BG:225:ALA:HB1 | 12:BG:226:PRO:HD2 | 2.02 | 0.41 |
| 1:BH:146:VAL:HG11 | 1:BH:172:ILE:HG12 | 2.01 | 0.41 |
| 1:BH:413:TYR:HB2 | 1:BH:639:LEU:O | 2.21 | 0.41 |
| 1:BI:158:ASN:ND2 | 1:BI:160:GLN:HG2 | 2.35 | 0.41 |
| 2:BJ:174:HIS:HB3 | 2:BJ:535:VAL:HB | 2.03 | 0.41 |
| 2:BJ:321:VAL:HA | 2:BJ:326:VAL:HA | 2.01 | 0.41 |
| 2:BJ:579:LYS:HE3 | 2:BJ:579:LYS:HB3 | 1.86 | 0.41 |
| 2:BJ:675:LEU:HA | 2:BJ:675:LEU:HD12 | 1.67 | 0.41 |
| 2:BJ:774:SER:OG | 2:BJ:835:GLU:O | 2.34 | 0.41 |
| 2:BJ:872:SER:HA | 2:BJ:875:TRP:CD1 | 2.55 | 0.41 |
| 2:BJ:899:PHE:O | 2:BJ:900:ILE:HD13 | 2.21 | 0.41 |
| 2:C:228:ARG:NH2 | 5:K:559:PRO:HD3 | 2.35 | 0.41 |
| 2:C:729:SER:OG | 2:C:730:ARG:N | 2.54 | 0.41 |
| 2:C:788:THR:OG1 | 2:C:789:ALA:N | 2.54 | 0.41 |
| 2:C:821:ILE:HD12 | 2:C:821:ILE:H | 1.85 | 0.41 |
| 2:C:904:LEU:HD12 | 2:C:905:THR:N | 2.36 | 0.41 |
| 3:CA:95:TRP:CZ2 | 3:CA:169:PRO:HD3 | 2.55 | 0.41 |
| 3:CA:237:GLY:O | 3:CA:240:TYR:N | 2.48 | 0.41 |
| 3:CA:248:ARG:HA | 3:CA:330:ILE:O | 2.20 | 0.41 |
| 4:CD:192:PHE:O | 4:CD:261:VAL:N | 2.51 | 0.41 |
| 4:CE:251:ASN:N | 4:CE:266:SER:O | 2.53 | 0.41 |
| 5:CF:450:PHE:CZ | 5:CF:454:TYR:HD2 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:94:ARG:CD | 5:CG:134:GLU:HG2 | 2.51 | 0.41 |
| 5:CG:138:CYS:SG | 5:CG:140:PRO:HD2 | 2.60 | 0.41 |
| 5:CG:532:LEU:HA | 5:CG:532:LEU:HD23 | 1.87 | 0.41 |
| 6:CI:109:VAL:HG13 | 6:CI:178:ILE:HG21 | 2.02 | 0.41 |
| 6:CI:195:LEU:HA | 6:CI:215:PHE:HD1 | 1.85 | 0.41 |
| 6:CJ:145:SER:O | 6:CJ:159:THR:N | 2.45 | 0.41 |
| 6:DA:47:PHE:HE2 | 6:DA:51:ASN:HB3 | 1.84 | 0.41 |
| 7:DB:173:ILE:HA | 7:DB:173:ILE:HD12 | 1.89 | 0.41 |
| 7:DB:29:ILE:CG2 | 7:DB:30:THR:H | 2.18 | 0.41 |
| 7:DB:503:ASN:ND2 | 7:DD:445:HIS:HB2 | 2.35 | 0.41 |
| 7:DB:87:TYR:HA | 7:FE:412:PRO:CG | 2.50 | 0.41 |
| 7:DB:262:VAL:HB | 7:DC:261:GLY:N | 2.35 | 0.41 |
| 7:DC:372:CYS:SG | 7:DC:525:VAL:HB | 2.60 | 0.41 |
| 7:DD:134:SER:N | 7:DD:142:ILE:HD11 | 2.35 | 0.41 |
| 7:DD:147:LEU:HB2 | 7:DD:148:PRO:HD3 | 2.02 | 0.41 |
| 9:DG:115:ASN:OD1 | 11:GB:47:THR:OG1 | 2.38 | 0.41 |
| 10:DH:338:LEU:HA | 10:DH:338:LEU:HD23 | 1.86 | 0.41 |
| 3:E:60:TYR:HA | 3:E:61:PRO:HD3 | 1.96 | 0.41 |
| 1:EA:243:ILE:HG22 | 1:EA:258:GLY:HA3 | 2.03 | 0.41 |
| 1:EA:609:ILE:HG22 | 1:EA:611:LEU:HG | 2.01 | 0.41 |
| 1:EA:23:GLY:HA2 | 1:EA:68:GLN:NE2 | 2.35 | 0.41 |
| 1:EB:485:VAL:HG22 | 1:EB:624:TYR:CD1 | 2.55 | 0.41 |
| 1:EB:611:LEU:HD11 | 1:EB:616:PHE:CE2 | 2.54 | 0.41 |
| 2:EC:217:GLN:HG2 | 2:EC:218:THR:H | 1.85 | 0.41 |
| 2:EC:224:LEU:O | 2:EC:224:LEU:HD23 | 2.21 | 0.41 |
| 2:EC:514:PHE:HD1 | 2:EC:525:TRP:HB2 | 1.85 | 0.41 |
| 2:EC:740:ILE:O | 2:EC:743:SER:HB3 | 2.20 | 0.41 |
| 4:EF:173:SER:N | 4:EG:166:SER:OG | 2.39 | 0.41 |
| 5:EI:103:ASN:CG | 5:EI:104:VAL:H | 2.24 | 0.41 |
| 5:EJ:94:ARG:CD | 5:EJ:134:GLU:HG2 | 2.51 | 0.41 |
| 5:EJ:137:TYR:HB2 | 5:EJ:143:TRP:HE1 | 1.85 | 0.41 |
| 5:EJ:290:SER:HA | 5:EJ:371:PHE:H | 1.85 | 0.41 |
| 5:EJ:38:GLY:HA2 | 5:EJ:43:PRO:HA | 2.02 | 0.41 |
| 5:EJ:454:TYR:HD1 | 5:EJ:458:THR:HG21 | 1.85 | 0.41 |
| 5:EJ:49:TRP:N | 5:EJ:49:TRP:CD1 | 2.87 | 0.41 |
| 5:EJ:49:TRP:CZ3 | 5:EJ:96:ARG:HD2 | 2.52 | 0.41 |
| 4:F:124:ILE:HB | 4:F:137:LEU:HB3 | 2.01 | 0.41 |
| 5:FA:117:ILE:HG22 | 5:FA:143:TRP:HB2 | 2.02 | 0.41 |
| 7:O:467:ASN:ND2 | 5:FA:351:GLN:HG2 | 2.35 | 0.41 |
| 5:FA:258:TYR:HD1 | 5:FA:386:PHE:HD1 | 1.66 | 0.41 |
| 5:EI:402:GLU:HG2 | 5:FA:396:LYS:HE3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:FB:88:TRP:HB3 | 6:FB:90:PHE:CE1 | 2.55 | 0.41 |
| 6:FC:90:PHE:CD2 | 6:FC:126:VAL:HG22 | 2.45 | 0.41 |
| 7:FE:134:SER:H | 7:FE:142:ILE:CD1 | 2.33 | 0.41 |
| 7:FG:101:SER:OG | 7:FG:102:THR:N | 2.52 | 0.41 |
| 7:FF:117:THR:HB | 7:FG:112:ASN:HA | 2.01 | 0.41 |
| 7:FG:196:VAL:HG22 | 7:FG:214:THR:HG22 | 2.02 | 0.41 |
| 7:FG:73:THR:HG23 | 7:FG:74:LYS:N | 2.36 | 0.41 |
| 8:FH:53:PHE:HB2 | 12:GC:7:PHE:CE2 | 2.55 | 0.41 |
| 4:G:224:ASP:OD2 | 4:G:227:ASN:HB2 | 2.19 | 0.41 |
| 10:GA:62:LEU:O | 10:GA:128:LEU:HD12 | 2.20 | 0.41 |
| 11:GB:177:ILE:HG23 | 11:GB:178:ASN:N | 2.35 | 0.41 |
| 12:GC:196:GLU:HG2 | 12:GC:218:MET:O | 2.21 | 0.41 |
| 1:GD:205:GLU:O | 1:GD:206:TRP:HD1 | 2.04 | 0.41 |
| 1:GD:377:LYS:HD3 | 1:GD:641:VAL:HG21 | 2.02 | 0.41 |
| 1:GD:69:GLN:HE21 | 11:IE:25:MET:HE1 | 1.85 | 0.41 |
| 1:GE:158:ASN:ND2 | 1:GE:160:GLN:HG2 | 2.35 | 0.41 |
| 1:GE:189:ASP:O | 1:GE:192:ILE:HG23 | 2.20 | 0.41 |
| 1:GE:240:GLU:HB2 | 2:GF:719:LYS:HZ1 | 1.85 | 0.41 |
| 1:GE:347:THR:OG1 | 1:GE:348:PHE:N | 2.54 | 0.41 |
| 2:GF:224:LEU:O | 2:GF:224:LEU:HD23 | 2.21 | 0.41 |
| 2:GF:33:TYR:CE1 | 2:GF:85:ALA:HB3 | 2.55 | 0.41 |
| 2:GF:580:LYS:HG2 | 2:GF:581:TYR:N | 2.22 | 0.41 |
| 2:GF:740:ILE:O | 2:GF:743:SER:HB3 | 2.20 | 0.41 |
| 3:GG:131:TYR:HD1 | 3:GG:190:TYR:HA | 1.84 | 0.41 |
| 4:HA:192:PHE:O | 4:HA:261:VAL:N | 2.51 | 0.41 |
| 5:HB:331:CYS:HA | 5:HB:349:TRP:CZ2 | 2.46 | 0.41 |
| 5:HB:67:SER:HA | 5:HB:94:ARG:O | 2.20 | 0.41 |
| 5:HC:344:VAL:O | 5:HC:345:LEU:HD12 | 2.21 | 0.41 |
| 5:HD:304:ILE:HD12 | 5:HD:306:PRO:HA | 2.02 | 0.41 |
| 6:HF:109:VAL:HG13 | 6:HF:178:ILE:HG21 | 2.03 | 0.41 |
| 7:HJ:232:THR:CG2 | 7:HJ:235:GLU:H | 2.34 | 0.41 |
| 5:I:118:LYS:HA | 5:I:142:ARG:NH2 | 2.35 | 0.41 |
| 11:IE:133:TRP:CE2 | 11:IE:150:LEU:HD11 | 2.55 | 0.41 |
| 11:IE:146:TYR:HE2 | 11:IE:150:LEU:HD23 | 1.85 | 0.41 |
| 12:IF:15:ASP:CG | 12:IF:16:PHE:N | 2.71 | 0.41 |
| 5:J:454:TYR:HD1 | 5:J:458:THR:HG21 | 1.85 | 0.41 |
| 5:J:559:PRO:HA | 5:J:561:GLU:OE2 | 2.21 | 0.41 |
| 5:J:54:ALA:HB2 | 5:J:71:ASN:O | 2.20 | 0.41 |
| 5:K:323:THR:CG2 | 5:K:359:GLU:HB2 | 2.46 | 0.41 |
| 5:K:399:ILE:O | 5:K:402:GLU:HB3 | 2.20 | 0.41 |
| 5:K:89:TYR:CE1 | 5:K:137:TYR:CZ | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:L:164:GLN:NE2 | 6:N:57:ASN:HB2 | 2.35 | 0.41 |
| 6:L:195:LEU:HA | 6:L:215:PHE:HD1 | 1.86 | 0.41 |
| 6:L:88:TRP:HB3 | 6:L:90:PHE:CE1 | 2.55 | 0.41 |
| 6:M:88:TRP:HB3 | 6:M:90:PHE:CE1 | 2.55 | 0.41 |
| 6:N:109:VAL:HG13 | 6:N:178:ILE:HG21 | 2.02 | 0.41 |
| 7:O:125:LEU:O | 7:O:129:PHE:N | 2.45 | 0.41 |
| 7:O:176:ILE:HG12 | 7:O:177:ALA:N | 2.33 | 0.41 |
| 7:P:372:CYS:SG | 7:P:525:VAL:HB | 2.60 | 0.41 |
| 7:P:358:ALA:HB1 | 7:P:524:LYS:HE3 | 2.02 | 0.41 |
| 7:Q:110:VAL:HG12 | 7:Q:111:ASN:H | 1.84 | 0.41 |
| 7:O:76:VAL:N | 7:Q:76:VAL:O | 2.34 | 0.41 |
| 11:V:71:TRP:O | 11:V:74:LEU:N | 2.53 | 0.41 |
| 12:W:187:GLY:C | 12:W:188:LEU:HD12 | 2.40 | 0.41 |
| 12:W:18:ARG:HB2 | 12:W:21:MET:HG2 | 2.01 | 0.41 |
| 1:X:205:GLU:O | 1:X:206:TRP:HD1 | 2.04 | 0.41 |
| 1:X:175:THR:O | 1:X:270:ILE:HG22 | 2.20 | 0.41 |
| 1:X:315:GLY:HA2 | 1:X:356:ILE:CD1 | 2.50 | 0.41 |
| 1:X:485:VAL:HG22 | 1:X:624:TYR:CD1 | 2.53 | 0.41 |
| 1:Y:352:ARG:O | 1:Y:353:PHE:HB2 | 2.21 | 0.41 |
| 13:YA:187[D]:ARG:HD3 | 13:YA:187[D]:ARG:HA | 1.86 | 0.41 |
| 13:YA:293[A]:ASN:HA | 13:YA:296[A]:LEU:HB2 | 2.01 | 0.41 |
| 13:YA:293[F]:ASN:HA | 13:YA:296[F]:LEU:HB2 | 2.02 | 0.41 |
| 13:YA:38[E]:GLN:O | 13:YA:46[E]:GLY:HA2 | 2.20 | 0.41 |
| 13:YA:410[D]:GLU:O | 13:YA:426[D]:PRO:HA | 2.20 | 0.41 |
| 13:YA:410[E]:GLU:O | 13:YA:426[E]:PRO:HA | 2.21 | 0.41 |
| 13:YA:439[D]:TYR:HB3 | 13:YA:441[D]:ILE:CD1 | 2.50 | 0.41 |
| 13:YA:445[A]:ASP:HA | 13:YC:453[A]:ASP:O | 2.20 | 0.41 |
| 13:YA:445[F]:ASP:HA | 13:YC:453[F]:ASP:O | 2.21 | 0.41 |
| 13:YA:530[F]:VAL:O | 13:YC:538[F]:VAL:HA | 2.20 | 0.41 |
| 13:YB:131[F]:VAL:O | 13:YB:134[F]:GLN:N | 2.46 | 0.41 |
| 13:YB:209[B]:GLN:HB3 | 13:YB:211[B]:VAL:HG23 | 2.03 | 0.41 |
| 13:YB:209[F]:GLN:HB3 | 13:YB:211[F]:VAL:HG23 | 2.02 | 0.41 |
| 13:YB:239[E]:GLU:H | 13:YB:239[E]:GLU:CD | 2.24 | 0.41 |
| 13:YB:239[D]:GLU:H | 13:YB:239[D]:GLU:CD | 2.24 | 0.41 |
| 13:YB:26[D]:ARG:HD3 | 14:YE:259[D]:LEU:HD21 | 2.01 | 0.41 |
| 13:YB:450[F]:VAL:HG11 | 13:YC:446[F]:GLY:H | 1.85 | 0.41 |
| 13:YB:552[D]:GLU:CB | 13:YC:544[D]:TRP:HB2 | 2.51 | 0.41 |
| 13:YB:76[D]:PRO:HB2 | 13:YB:98[D]:GLY:CA | 2.51 | 0.41 |
| 13:YC:209[D]:GLN:HB3 | 13:YC:211[D]:VAL:HG23 | 2.02 | 0.41 |
| 13:YC:209[F]:GLN:HB3 | 13:YC:211[F]:VAL:HG23 | 2.02 | 0.41 |
| 13:YC:293[F]:ASN:HA | 13:YC:296[F]:LEU:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:410[F]:GLU:O | 13:YC:426[F]:PRO:HA | 2.20 | 0.41 |
| 13:YB:436[D]:ASP:HB3 | 13:YC:429[D]:ARG:HA | 2.03 | 0.41 |
| 13:YA:553[A]:LYS:HA | 13:YC:560[A]:ILE:O | 2.21 | 0.41 |
| 14:YD:124[D]:PHE:CZ | 14:YD:135[D]:MET:HG2 | 2.55 | 0.41 |
| 14:YD:174[A]:ARG:CG | 14:YD:188[A]:VAL:HG22 | 2.51 | 0.41 |
| 14:YD:174[C]:ARG:CG | 14:YD:188[C]:VAL:HG22 | 2.51 | 0.41 |
| 14:YD:174[D]:ARG:CG | 14:YD:188[D]:VAL:HG22 | 2.51 | 0.41 |
| 14:YD:174[E]:ARG:CG | 14:YD:188[E]:VAL:HG22 | 2.51 | 0.41 |
| 14:YD:174[F]:ARG:CG | 14:YD:188[F]:VAL:HG22 | 2.51 | 0.41 |
| 14:YD:212[E]:ILE:HG12 | 14:YD:228[E]:TYR:HB2 | 2.03 | 0.41 |
| 14:YD:238[D]:THR:N | 14:YD:307[D]:TYR:O | 2.53 | 0.41 |
| 14:YD:238[E]:THR:N | 14:YD:307[E]:TYR:O | 2.53 | 0.41 |
| 14:YD:47[E]:ARG:NH1 | 14:YD:341[E]:GLU:OE1 | 2.53 | 0.41 |
| 14:YD:10[D]:PRO:HB2 | 14:YD:74[D]:VAL:HG21 | 2.03 | 0.41 |
| 14:YE:174[A]:ARG:CG | 14:YE:188[A]:VAL:HG22 | 2.51 | 0.41 |
| 14:YE:174[F]:ARG:CG | 14:YE:188[F]:VAL:HG22 | 2.51 | 0.41 |
| 14:YE:43[B]:SER:O | 14:YE:189[B]:TRP:HB2 | 2.20 | 0.41 |
| 14:YE:86[B]:ARG:HD2 | 14:YE:192[B]:ILE:HD12 | 2.01 | 0.41 |
| 14:YE:212[A]:ILE:HG12 | 14:YE:228[A]:TYR:HB2 | 2.02 | 0.41 |
| 14:YE:345[D]:GLU:HB3 | 14:YE:352[D]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:38[D]:LEU:HA | 14:YE:38[D]:LEU:HD12 | 1.63 | 0.41 |
| 14:YE:10[C]:PRO:HB2 | 14:YE:74[C]:VAL:HG21 | 2.03 | 0.41 |
| 14:YF:112[B]:ILE:HB | 14:YF:140[B]:TYR:OH | 2.20 | 0.41 |
| 14:YF:230[B]:LEU:HD13 | 14:YF:230[B]:LEU:HA | 1.84 | 0.41 |
| 14:YD:91[C]:LYS:O | 14:YF:242[C]:PRO:HD2 | 2.20 | 0.41 |
| 14:YF:238[F]:THR:N | 14:YF:307[F]:TYR:O | 2.53 | 0.41 |
| 2:Z:314:THR:HG23 | 2:Z:317:TYR:HB2 | 2.01 | 0.41 |
| 2:Z:425:ARG:NH2 | 2:Z:449:LYS:HG2 | 2.36 | 0.41 |
| 2:Z:584:GLY:HA2 | 2:Z:600:PHE:CB | 2.46 | 0.41 |
| 2:Z:904:LEU:HD12 | 2:Z:905:THR:N | 2.36 | 0.41 |
| 1:A:111:MET:O | 1:A:111:MET:HG3 | 2.20 | 0.41 |
| 1:A:205:GLU:O | 1:A:206:TRP:HD1 | 2.04 | 0.41 |
| 1:A:278:ALA:HB2 | 1:A:317:GLY:N | 2.33 | 0.41 |
| 4:AA:17:ASN:OD1 | 4:AA:18:ALA:N | 2.53 | 0.41 |
| 4:AA:172:GLU:OE1 | 4:AB:164:ILE:HG23 | 2.20 | 0.41 |
| 4:AB:251:ASN:N | 4:AB:266:SER:O | 2.53 | 0.41 |
| 5:AC:271:THR:HB | 5:AC:273:LYS:HG2 | 2.03 | 0.41 |
| 5:AC:304:ILE:HG21 | 5:AC:309:LEU:HD12 | 2.01 | 0.41 |
| 5:AC:319:GLU:HG3 | 5:AD:262:GLN:OE1 | 2.19 | 0.41 |
| 5:AC:450:PHE:CZ | 5:AC:454:TYR:HD2 | 2.38 | 0.41 |
| 5:AD:48:ALA:C | 5:AD:49:TRP:CD1 | 2.93 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AC:572:ALA:HA | 5:AD:540:GLU:HG2 | 2.02 | 0.41 |
| 5:AE:357:SER:N | 5:AE:372:ASP:OD1 | 2.54 | 0.41 |
| 5:AE:89:TYR:CE1 | 5:AE:137:TYR:CZ | 3.09 | 0.41 |
| 6:AH:109:VAL:HG13 | 6:AH:178:ILE:HG21 | 2.02 | 0.41 |
| 7:AI:212:PRO:HA | 7:AI:215:PHE:HB3 | 2.02 | 0.41 |
| 7:AI:227:VAL:HG23 | 7:AJ:225:LYS:HB3 | 2.03 | 0.41 |
| 7:AI:255:SER:N | 7:AI:278:SER:OG | 2.53 | 0.41 |
| 7:AI:77:THR:HG23 | 7:AI:79:ALA:H | 1.85 | 0.41 |
| 7:AJ:250:LEU:HD23 | 7:BA:253:ARG:HH11 | 1.85 | 0.41 |
| 7:AI:251:ASN:HB2 | 7:AJ:253:ARG:HH22 | 1.85 | 0.41 |
| 1:B:145:PHE:CD1 | 1:B:169:GLN:HA | 2.56 | 0.41 |
| 1:B:322:ILE:O | 1:B:325:ILE:HB | 2.21 | 0.41 |
| 1:B:33:LEU:HD12 | 1:B:33:LEU:HA | 1.89 | 0.41 |
| 1:B:565:GLU:OE1 | 1:B:571:PRO:HD3 | 2.20 | 0.41 |
| 7:AJ:75:ALA:HB1 | 7:BA:75:ALA:HB1 | 2.03 | 0.41 |
| 8:BC:88:TRP:CE3 | 8:BC:134:PRO:HD3 | 2.53 | 0.41 |
| 10:BE:286:VAL:H | 14:YF:215[E]:GLU:CD | 2.23 | 0.41 |
| 1:BH:491:PHE:CE2 | 1:BH:619:GLN:HA | 2.55 | 0.41 |
| 1:BI:209:TRP:O | 1:BI:210:THR:C | 2.58 | 0.41 |
| 1:BI:257:ILE:HG22 | 1:BI:258:GLY:N | 2.36 | 0.41 |
| 1:BI:322:ILE:O | 1:BI:325:ILE:HB | 2.21 | 0.41 |
| 2:BJ:1019:PRO:HG3 | 3:CA:93:ARG:HD3 | 2.02 | 0.41 |
| 2:BJ:108:TYR:N | 2:BJ:108:TYR:CD2 | 2.87 | 0.41 |
| 2:BJ:151:PHE:HB3 | 2:BJ:166:PHE:CZ | 2.56 | 0.41 |
| 2:BJ:253:ILE:HG13 | 2:BJ:300:LEU:CD2 | 2.51 | 0.41 |
| 2:BJ:516:TRP:HE1 | 2:BJ:518:LYS:HG2 | 1.85 | 0.41 |
| 2:BJ:584:GLY:CA | 2:BJ:600:PHE:HB3 | 2.48 | 0.41 |
| 2:BJ:81:ARG:HG2 | 2:BJ:94:TRP:CE3 | 2.51 | 0.41 |
| 2:BJ:33:TYR:CE1 | 2:BJ:85:ALA:HB3 | 2.55 | 0.41 |
| 2:C:28:VAL:HG23 | 2:C:29:GLY:N | 2.35 | 0.41 |
| 2:C:618:PHE:CD1 | 2:C:619:LEU:HB2 | 2.55 | 0.41 |
| 2:C:740:ILE:O | 2:C:743:SER:HB3 | 2.20 | 0.41 |
| 2:C:752:TYR:O | 2:C:753:ASN:OD1 | 2.39 | 0.41 |
| 3:CB:150:LYS:HG3 | 3:CB:160:TRP:CG | 2.55 | 0.41 |
| 3:CB:80:LYS:HG2 | 3:CB:81:VAL:H | 1.85 | 0.41 |
| 4:CC:173:SER:N | 4:CD:166:SER:OG | 2.41 | 0.41 |
| 5:CF:185:SER:HB2 | 5:CF:228:PHE:HE1 | 1.84 | 0.41 |
| 5:CF:204:ASP:OD1 | 5:CF:205:VAL:N | 2.50 | 0.41 |
| 5:CF:322:GLY:N | 5:CF:360:THR:HG23 | 2.35 | 0.41 |
| 5:CG:102:TRP:HE3 | 5:CG:131:SER:HB2 | 1.84 | 0.41 |
| 5:CG:290:SER:HA | 5:CG:371:PHE:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CF:472:TYR:O | 5:CG:416:ILE:HD12 | 2.20 | 0.41 |
| 5:CH:192:ARG:CG | 5:CH:245:GLU:HB2 | 2.50 | 0.41 |
| 5:CH:215:PRO:HB3 | 5:CH:229:ASN:C | 2.40 | 0.41 |
| 5:CH:390:LEU:HD23 | 5:CH:391:GLY:N | 2.36 | 0.41 |
| 5:CH:497:PRO:HG2 | 5:CH:498:ASN:HD22 | 1.86 | 0.41 |
| 3:D:96:GLY:HA2 | 3:D:103:PRO:CB | 2.50 | 0.41 |
| 3:D:114:CYS:HA | 3:D:120:ASN:HD21 | 1.85 | 0.41 |
| 3:D:71:MET:HG2 | 3:D:309:MET:CE | 2.51 | 0.41 |
| 7:DB:197:ALA:O | 7:DB:201:GLN:HG3 | 2.20 | 0.41 |
| 7:DC:358:ALA:HB1 | 7:DC:524:LYS:HE3 | 2.02 | 0.41 |
| 7:DD:196:VAL:HG22 | 7:DD:214:THR:HG22 | 2.02 | 0.41 |
| 7:DC:227:VAL:CG2 | 7:DD:225:LYS:HB3 | 2.49 | 0.41 |
| 7:DC:347:MET:HE1 | 7:DD:345:ALA:HB1 | 2.02 | 0.41 |
| 12:BG:143:TYR:CE1 | 10:DH:214:ARG:HD3 | 2.54 | 0.41 |
| 11:DI:177:ILE:HG23 | 11:DI:178:ASN:N | 2.35 | 0.41 |
| 12:DJ:225:ALA:HB1 | 12:DJ:226:PRO:HD2 | 2.02 | 0.41 |
| 3:D:316:PRO:HG2 | 3:E:6:VAL:HG13 | 2.02 | 0.41 |
| 1:EA:418:THR:HG22 | 1:EA:482:ILE:HG22 | 2.02 | 0.41 |
| 1:EB:322:ILE:O | 1:EB:325:ILE:HB | 2.21 | 0.41 |
| 1:EB:543:THR:HG1 | 1:EB:544:ASP:N | 2.17 | 0.41 |
| 2:EC:411:LYS:O | 2:EC:412:THR:HB | 2.21 | 0.41 |
| 2:EC:431:TYR:HB3 | 2:EC:485:TYR:OH | 2.20 | 0.41 |
| 2:EC:103:PHE:CZ | 2:EC:627:GLU:HA | 2.56 | 0.41 |
| 2:EC:872:SER:HA | 2:EC:875:TRP:CD1 | 2.55 | 0.41 |
| 2:EC:884:HIS:CG | 2:EC:885:PRO:HD2 | 2.56 | 0.41 |
| 2:EC:947:VAL:HB | 3:ED:119:TYR:HD2 | 1.86 | 0.41 |
| 3:EE:60:TYR:HA | 3:EE:61:PRO:HD3 | 1.96 | 0.41 |
| 4:EF:82:GLY:O | 4:EH:64:THR:N | 2.38 | 0.41 |
| 4:EG:205:THR:OG1 | 4:EH:199:MET:SD | 2.79 | 0.41 |
| 4:EG:60:ILE:HB | 4:EH:4:GLN:NE2 | 2.36 | 0.41 |
| 5:EI:137:TYR:HA | 5:EI:143:TRP:CD1 | 2.55 | 0.41 |
| 5:EI:137:TYR:HA | 5:EI:143:TRP:HD1 | 1.84 | 0.41 |
| 5:EI:151:ILE:O | 5:EI:152:ASP:HB3 | 2.21 | 0.41 |
| 5:EI:271:THR:HB | 5:EI:273:LYS:HG2 | 2.03 | 0.41 |
| 5:EI:323:THR:CG2 | 5:EI:359:GLU:HB2 | 2.48 | 0.41 |
| 5:EJ:139:ALA:HB3 | 5:EJ:140:PRO:HD3 | 2.01 | 0.41 |
| 5:FA:118:LYS:HA | 5:FA:142:ARG:CZ | 2.51 | 0.41 |
| 5:FA:357:SER:N | 5:FA:372:ASP:OD1 | 2.54 | 0.41 |
| 5:FA:507:ASP:OD1 | 5:FA:510:GLY:N | 2.53 | 0.41 |
| 6:FB:164:GLN:NE2 | 6:FD:57:ASN:HB2 | 2.35 | 0.41 |
| 7:FE:478:ASP:N | 7:FE:478:ASP:OD1 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:87:TYR:HA | 7:HH:412:PRO:HG2 | 2.02 | 0.41 |
| 7:FF:433:TYR:CE2 | 7:FF:436:GLU:HB2 | 2.56 | 0.41 |
| 7:FF:458:GLY:O | 7:FF:461:GLY:N | 2.41 | 0.41 |
| 7:FG:20:PRO:CG | 7:FG:29:ILE:HG13 | 2.49 | 0.41 |
| 8:FH:91:ILE:HG22 | 8:FH:107:TYR:HB3 | 2.02 | 0.41 |
| 8:FI:91:ILE:HG22 | 8:FI:107:TYR:HB3 | 2.01 | 0.41 |
| 8:FI:10:PHE:CE1 | 8:IB:35:GLN:HG2 | 2.55 | 0.41 |
| 9:FJ:62:PHE:HZ | 9:FJ:127:ALA:HA | 1.86 | 0.41 |
| 4:F:32:ASN:HD21 | 4:G:10:ILE:HB | 1.84 | 0.41 |
| 10:GA:62:LEU:HA | 10:GA:62:LEU:HD12 | 1.88 | 0.41 |
| 11:GB:71:TRP:O | 11:GB:74:LEU:N | 2.53 | 0.41 |
| 12:GC:15:ASP:O | 12:GC:16:PHE:CD1 | 2.73 | 0.41 |
| 1:GD:315:GLY:HA2 | 1:GD:356:ILE:CD1 | 2.50 | 0.41 |
| 1:GD:360:VAL:HG23 | 1:GD:375:ALA:O | 2.20 | 0.41 |
| 1:GE:145:PHE:CD1 | 1:GE:169:GLN:HA | 2.56 | 0.41 |
| 1:GE:257:ILE:HG22 | 1:GE:258:GLY:N | 2.36 | 0.41 |
| 1:GE:322:ILE:O | 1:GE:325:ILE:HB | 2.21 | 0.41 |
| 2:GF:151:PHE:HB3 | 2:GF:166:PHE:CZ | 2.56 | 0.41 |
| 2:GF:28:VAL:HG23 | 2:GF:29:GLY:N | 2.35 | 0.41 |
| 2:GF:31:ASN:O | 2:GF:32:PHE:HD1 | 2.04 | 0.41 |
| 2:GF:431:TYR:HB3 | 2:GF:485:TYR:OH | 2.20 | 0.41 |
| 3:GG:138:ASP:HA | 3:GG:150:LYS:HE3 | 2.03 | 0.41 |
| 3:GG:95:TRP:CZ2 | 3:GG:169:PRO:HD3 | 2.55 | 0.41 |
| 2:GF:912:ILE:HD11 | 3:GG:329:ASN:HB2 | 2.03 | 0.41 |
| 3:GG:57:ALA:HB2 | 3:GH:7:ILE:HG12 | 2.03 | 0.41 |
| 4:GI:251:ASN:N | 4:GI:266:SER:O | 2.53 | 0.41 |
| 4:GJ:213:LYS:HE3 | 4:GJ:249:ILE:HG12 | 2.03 | 0.41 |
| 4:GJ:54:THR:HA | 4:HA:7:LYS:O | 2.20 | 0.41 |
| 5:HB:572:ALA:HA | 5:HC:540:GLU:HG2 | 2.03 | 0.41 |
| 5:HD:303:PRO:HD2 | 5:HD:365:ILE:HD13 | 2.02 | 0.41 |
| 5:HD:258:TYR:HD1 | 5:HD:386:PHE:HD1 | 1.66 | 0.41 |
| 5:HD:409:SER:OG | 5:HD:411:GLY:N | 2.52 | 0.41 |
| 7:HH:143:LYS:HG2 | 7:HI:138:SER:C | 2.40 | 0.41 |
| 7:HH:176:ILE:HG12 | 7:HH:177:ALA:N | 2.33 | 0.41 |
| 7:HH:439:ILE:HG12 | 7:HJ:515:TRP:CZ3 | 2.56 | 0.41 |
| 6:FB:213:TYR:OH | 7:HI:171:LYS:HG3 | 2.19 | 0.41 |
| 7:HH:190:VAL:HB | 7:HI:189:GLY:N | 2.36 | 0.41 |
| 7:HI:232:THR:O | 7:HI:236:VAL:HG22 | 2.20 | 0.41 |
| 7:HI:26:PRO:HA | 7:HI:27:PRO:HD3 | 1.72 | 0.41 |
| 7:HI:453:GLU:HG3 | 7:HI:475:LEU:HD11 | 2.03 | 0.41 |
| 7:HH:503:ASN:ND2 | 7:HJ:446:LYS:H | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:104:VAL:HG22 | 5:I:105:ASN:H | 1.86 | 0.41 |
| 5:I:103:ASN:CG | 5:I:104:VAL:H | 2.24 | 0.41 |
| 8:IB:89:GLN:HB3 | 8:IB:134:PRO:CG | 2.50 | 0.41 |
| 12:GC:153:ARG:NH2 | 12:IF:184:PRO:HA | 2.35 | 0.41 |
| 5:J:104:VAL:HG13 | 5:J:105:ASN:H | 1.84 | 0.41 |
| 6:N:168:LEU:HD23 | 6:N:168:LEU:HA | 4.27 | 0.41 |
| 7:O:212:PRO:HA | 7:O:215:PHE:HB3 | 2.02 | 0.41 |
| 7:O:44:VAL:HG21 | 7:P:25:PHE:HB3 | 2.03 | 0.41 |
| 7:O:227:VAL:HG23 | 7:P:225:LYS:HD3 | 2.02 | 0.41 |
| 7:P:232:THR:O | 7:P:236:VAL:HG22 | 2.20 | 0.41 |
| 7:O:445:HIS:NE2 | 7:P:447:HIS:CE1 | 2.89 | 0.41 |
| 7:Q:166:GLN:O | 7:Q:170:ILE:HB | 2.20 | 0.41 |
| 7:Q:232:THR:CG2 | 7:Q:235:GLU:H | 2.34 | 0.41 |
| 8:S:15:PHE:N | 8:S:15:PHE:CD1 | 2.84 | 0.41 |
| 1:X:111:MET:HG3 | 1:X:111:MET:O | 2.20 | 0.41 |
| 13:YA:209[B]:GLN:HB3 | 13:YA:211[B]:VAL:HG23 | 2.03 | 0.41 |
| 13:YA:239[A]:GLU:H | 13:YA:239[A]:GLU:CD | 2.24 | 0.41 |
| 13:YA:454[B]:LYS:C | 13:YA:455[B]:LYS:HG3 | 2.39 | 0.41 |
| 13:YA:47[B]:ILE:HG23 | 14:YD:123[B]:PRO:CG | 2.48 | 0.41 |
| 13:YA:47[D]:ILE:HG23 | 14:YD:123[D]:PRO:CG | 2.50 | 0.41 |
| 13:YA:47[F]:ILE:HG23 | 14:YD:123[F]:PRO:CG | 2.48 | 0.41 |
| 13:YA:530[E]:VAL:O | 13:YC:538[E]:VAL:HA | 2.19 | 0.41 |
| 13:YA:550[C]:TRP:HB2 | 13:YC:554[C]:MET:HG3 | 2.02 | 0.41 |
| 13:YA:76[B]:PRO:HB2 | 13:YA:98[B]:GLY:O | 2.21 | 0.41 |
| 13:YB:239[F]:GLU:H | 13:YB:239[F]:GLU:CD | 2.24 | 0.41 |
| 13:YB:24[C]:LEU:HA | 13:YB:24[C]:LEU:HD12 | 1.63 | 0.41 |
| 13:YB:38[A]:GLN:O | 13:YB:46[A]:GLY:HA2 | 2.20 | 0.41 |
| 13:YB:454[F]:LYS:C | 13:YB:455[F]:LYS:HG3 | 2.40 | 0.41 |
| 13:YB:515[F]:LYS:HG3 | 13:YC:507[F]:GLU:HA | 2.02 | 0.41 |
| 13:YB:552[C]:GLU:CB | 13:YC:544[C]:TRP:HB2 | 2.51 | 0.41 |
| 13:YB:76[A]:PRO:HB2 | 13:YB:98[A]:GLY:CA | 2.51 | 0.41 |
| 13:YC:219[A]:LYS:HE3 | 13:YC:219[A]:LYS:HB2 | 1.81 | 0.41 |
| 13:YC:239[B]:GLU:H | 13:YC:239[B]:GLU:CD | 2.24 | 0.41 |
| 13:YC:239[D]:GLU:H | 13:YC:239[D]:GLU:CD | 2.24 | 0.41 |
| 13:YC:410[B]:GLU:O | 13:YC:426[B]:PRO:HA | 2.21 | 0.41 |
| 13:YA:438[A]:LEU:CD2 | 13:YC:442[A]:THR:HG21 | 2.48 | 0.41 |
| 13:YA:463[B]:ILE:HA | 13:YC:471[B]:LEU:O | 2.20 | 0.41 |
| 13:YC:47[C]:ILE:HG23 | 14:YF:123[C]:PRO:CG | 2.48 | 0.41 |
| 13:YA:486[D]:GLU:CB | 13:YC:490[D]:VAL:HG11 | 2.51 | 0.41 |
| 13:YA:486[F]:GLU:CB | 13:YC:490[F]:VAL:HG11 | 2.51 | 0.41 |
| 13:YB:546[B]:VAL:HG11 | 13:YC:542[B]:VAL:HG13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:51[C]:MET:SD | 14:YD:108[C]:GLU:HA | 2.61 | 0.41 |
| 14:YD:51[D]:MET:SD | 14:YD:108[D]:GLU:HA | 2.61 | 0.41 |
| 14:YD:136[C]:LEU:HD21 | 14:YD:166[C]:PHE:CE2 | 2.56 | 0.41 |
| 14:YD:238[F]:THR:N | 14:YD:307[F]:TYR:O | 2.53 | 0.41 |
| 14:YD:38[F]:LEU:HA | 14:YD:38[F]:LEU:HD12 | 1.63 | 0.41 |
| 14:YD:75[E]:ALA:HB2 | 14:YD:83[E]:VAL:HA | 2.01 | 0.41 |
| 14:YE:51[A]:MET:SD | 14:YE:108[A]:GLU:HA | 2.61 | 0.41 |
| 14:YE:10[D]:PRO:HB2 | 14:YE:74[D]:VAL:HG21 | 2.03 | 0.41 |
| 14:YE:124[B]:PHE:CZ | 14:YE:135[B]:MET:HG2 | 2.55 | 0.41 |
| 14:YE:174[D]:ARG:CG | 14:YE:188[D]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:51[D]:MET:SD | 14:YF:108[D]:GLU:HA | 2.61 | 0.41 |
| 14:YF:174[B]:ARG:CG | 14:YF:188[B]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:174[E]:ARG:CG | 14:YF:188[E]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:212[E]:ILE:HG12 | 14:YF:228[E]:TYR:HB2 | 2.03 | 0.41 |
| 13:YA:100[C]:TYR:CD2 | 14:YF:258[C]:PHE:HD1 | 2.39 | 0.41 |
| 14:YF:238[B]:THR:N | 14:YF:307[B]:TYR:O | 2.53 | 0.41 |
| 14:YF:38[B]:LEU:HD12 | 14:YF:38[B]:LEU:HA | 1.63 | 0.41 |
| 2:Z:1012:LEU:HD12 | 2:Z:1012:LEU:O | 2.21 | 0.41 |
| 2:Z:618:PHE:CD1 | 2:Z:619:LEU:HB2 | 2.55 | 0.41 |
| 15:ZA:56[D]:HIS:CD2 | 15:ZA:83[D]:CYS:HB2 | 2.56 | 0.41 |
| 1:A:222:THR:C | 1:A:223:ILE:HG12 | 2.40 | 0.41 |
| 1:A:414:LEU:HD21 | 1:A:486:ARG:HH21 | 1.85 | 0.41 |
| 1:A:572:TYR:CE2 | 1:A:574:GLY:HA3 | 2.56 | 0.41 |
| 4:AA:65:GLY:HA3 | 4:AA:84:ARG:NH1 | 2.36 | 0.41 |
| 4:AA:113:ASN:ND2 | 4:AB:103:LEU:HD21 | 2.26 | 0.41 |
| 4:AB:65:GLY:HA3 | 4:AB:84:ARG:NH1 | 2.36 | 0.41 |
| 5:AC:258:TYR:CE1 | 5:AC:384:THR:HG23 | 2.55 | 0.41 |
| 5:AD:186:TYR:HB3 | 5:AD:227:GLY:O | 2.20 | 0.41 |
| 5:AD:344:VAL:O | 5:AD:345:LEU:HD12 | 2.21 | 0.41 |
| 5:AD:559:PRO:HA | 5:AD:561:GLU:OE2 | 2.21 | 0.41 |
| 5:AE:89:TYR:HA | 5:AE:137:TYR:CD2 | 2.55 | 0.41 |
| 5:AE:118:LYS:HA | 5:AE:142:ARG:CZ | 2.51 | 0.41 |
| 5:AE:117:ILE:HG22 | 5:AE:143:TRP:HB2 | 2.02 | 0.41 |
| 5:AE:186:TYR:HB3 | 5:AE:227:GLY:C | 2.39 | 0.41 |
| 5:AE:322:GLY:CA | 5:AE:359:GLU:HA | 2.50 | 0.41 |
| 5:AE:497:PRO:HG2 | 5:AE:498:ASN:ND2 | 2.35 | 0.41 |
| 6:AF:79:PRO:HD2 | 6:AF:193:TRP:CB | 2.51 | 0.41 |
| 6:AF:70:ILE:HD12 | 6:AF:196:LEU:HD11 | 2.03 | 0.41 |
| 7:AI:451:PHE:CE1 | 7:AI:470:GLY:HA2 | 2.56 | 0.41 |
| 7:AI:49:ASP:OD1 | 7:AI:50:ALA:N | 2.54 | 0.41 |
| 7:AI:51:SER:HB3 | 7:AI:54:THR:HB | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AJ:232:THR:O | 7:AJ:236:VAL:HG22 | 2.20 | 0.41 |
| 1:B:257:ILE:HG22 | 1:B:258:GLY:N | 2.36 | 0.41 |
| 1:B:220:THR:HA | 1:B:260:LEU:HD13 | 2.03 | 0.41 |
| 7:BA:32:VAL:O | 7:BA:36:ILE:HG12 | 2.20 | 0.41 |
| 7:AI:503:ASN:HD21 | 7:BA:446:LYS:H | 1.68 | 0.41 |
| 7:AJ:77:THR:HG21 | 7:BA:72:ASN:CG | 2.40 | 0.41 |
| 8:BB:134:PRO:HA | 8:BB:157:LEU:HD23 | 2.02 | 0.41 |
| 1:BH:55:VAL:O | 1:BH:58:ASP:HB3 | 2.20 | 0.41 |
| 1:BI:220:THR:HA | 1:BI:260:LEU:HD13 | 2.03 | 0.41 |
| 1:BI:331:ILE:HA | 1:BI:331:ILE:HD13 | 1.84 | 0.41 |
| 1:BI:66:TYR:O | 1:BI:69:GLN:N | 2.54 | 0.41 |
| 1:BI:88:SER:O | 1:BI:91:GLN:HB3 | 2.21 | 0.41 |
| 2:BJ:222:VAL:HG12 | 2:BJ:224:LEU:HB2 | 2.01 | 0.41 |
| 2:BJ:319:TYR:CD2 | 2:BJ:375:VAL:HG21 | 2.56 | 0.41 |
| 2:BJ:623:LEU:HA | 2:BJ:623:LEU:HD23 | 1.82 | 0.41 |
| 2:BJ:103:PHE:CZ | 2:BJ:627:GLU:HA | 2.56 | 0.41 |
| 2:BJ:821:ILE:HD12 | 2:BJ:821:ILE:H | 1.85 | 0.41 |
| 2:BJ:78:TYR:O | 2:BJ:99:GLU:HB2 | 2.21 | 0.41 |
| 2:C:146:LEU:HA | 2:C:585:MET:HA | 2.02 | 0.41 |
| 2:C:821:ILE:N | 2:C:824:GLN:NE2 | 2.69 | 0.41 |
| 3:CA:79:VAL:HG12 | 3:CA:80:LYS:O | 2.21 | 0.41 |
| 4:CC:190:PRO:HA | 4:CC:262:THR:HA | 2.01 | 0.41 |
| 4:CC:213:LYS:HE3 | 4:CC:249:ILE:HG12 | 2.03 | 0.41 |
| 4:CD:213:LYS:HE3 | 4:CD:249:ILE:HG12 | 2.03 | 0.41 |
| 4:CE:65:GLY:HA3 | 4:CE:84:ARG:NH1 | 2.36 | 0.41 |
| 5:CF:118:LYS:HA | 5:CF:142:ARG:NH2 | 2.35 | 0.41 |
| 5:CF:162:VAL:HA | 5:CF:246:THR:O | 2.20 | 0.41 |
| 5:CG:344:VAL:O | 5:CG:345:LEU:HD12 | 2.21 | 0.41 |
| 5:CF:90:ASN:OD1 | 5:CG:49:TRP:HB2 | 2.21 | 0.41 |
| 5:CG:542:LEU:HD11 | 5:CH:569:TYR:HE2 | 1.82 | 0.41 |
| 5:CH:181:PHE:HE2 | 5:CH:246:THR:HG22 | 1.85 | 0.41 |
| 5:CH:507:ASP:OD1 | 5:CH:510:GLY:N | 2.53 | 0.41 |
| 5:CF:555:CYS:O | 5:CH:557:TYR:HE1 | 2.03 | 0.41 |
| 6:DA:82:VAL:HG23 | 6:DA:187:LYS:HE3 | 2.01 | 0.41 |
| 7:DC:99:ARG:HH11 | 7:DC:111:ASN:ND2 | 2.17 | 0.41 |
| 7:DC:183:ALA:HB2 | 7:DC:189:GLY:O | 2.20 | 0.41 |
| 5:CH:196:ARG:HH11 | 7:DC:8:HIS:HB3 | 1.85 | 0.41 |
| 8:BC:15:PHE:CB | 8:DF:150:ILE:HD11 | 2.51 | 0.41 |
| 10:DH:62:LEU:O | 10:DH:128:LEU:HD12 | 2.20 | 0.41 |
| 3:E:150:LYS:HG3 | 3:E:160:TRP:CG | 2.55 | 0.41 |
| 3:E:21:MET:HG3 | 3:E:247:ILE:HG13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:12:ARG:O | 2:EC:709:TYR:OH | 2.23 | 0.41 |
| 1:EA:448:TYR:CE2 | 1:EA:642:PHE:HB2 | 2.55 | 0.41 |
| 1:EA:580:LEU:HD12 | 1:EA:580:LEU:C | 2.41 | 0.41 |
| 1:EA:413:TYR:HB2 | 1:EA:639:LEU:O | 2.21 | 0.41 |
| 1:EB:240:GLU:CD | 1:EB:240:GLU:H | 2.22 | 0.41 |
| 1:EB:220:THR:HA | 1:EB:260:LEU:HD13 | 2.03 | 0.41 |
| 2:EC:174:HIS:HB3 | 2:EC:535:VAL:HB | 2.02 | 0.41 |
| 2:EC:186:ASP:HB3 | 2:EC:189:ARG:HG3 | 2.03 | 0.41 |
| 2:EC:412:THR:OG1 | 2:EC:413:TRP:N | 2.53 | 0.41 |
| 2:EC:540:LYS:HA | 2:EC:540:LYS:HD2 | 1.91 | 0.41 |
| 2:EC:821:ILE:H | 2:EC:821:ILE:HD12 | 1.85 | 0.41 |
| 2:EC:78:TYR:O | 2:EC:99:GLU:HB2 | 2.21 | 0.41 |
| 3:ED:255:SER:O | 3:ED:258:PHE:N | 2.53 | 0.41 |
| 4:EF:164:ILE:HG23 | 4:EH:172:GLU:OE1 | 2.20 | 0.41 |
| 4:EF:172:GLU:HA | 4:EG:166:SER:N | 2.36 | 0.41 |
| 5:EI:304:ILE:HG21 | 5:EI:309:LEU:HD12 | 2.01 | 0.41 |
| 5:EJ:102:TRP:HE3 | 5:EJ:131:SER:HB2 | 1.84 | 0.41 |
| 5:EJ:460:TYR:CE1 | 5:FA:458:THR:HG23 | 2.55 | 0.41 |
| 5:EJ:552:VAL:HG22 | 5:EJ:553:GLY:N | 2.36 | 0.41 |
| 5:FA:213:GLY:HA2 | 5:FA:221:GLU:HB2 | 2.02 | 0.41 |
| 5:FA:311:VAL:HA | 5:FA:382:ASN:O | 2.20 | 0.41 |
| 5:FA:390:LEU:HD23 | 5:FA:391:GLY:N | 2.36 | 0.41 |
| 5:FA:399:ILE:O | 5:FA:402:GLU:HB3 | 2.20 | 0.41 |
| 5:FA:318:GLN:NE2 | 6:FC:7:LYS:HB3 | 2.35 | 0.41 |
| 6:FC:54:SER:CA | 6:FD:164:GLN:HE22 | 2.34 | 0.41 |
| 7:FE:146:SER:N | 7:FE:149:GLN:HB2 | 2.35 | 0.41 |
| 7:FE:190:VAL:HG23 | 7:FF:188:GLN:HB3 | 2.01 | 0.41 |
| 7:FF:227:VAL:CG2 | 7:FG:225:LYS:HB3 | 2.50 | 0.41 |
| 7:FF:372:CYS:SG | 7:FF:525:VAL:HB | 2.60 | 0.41 |
| 4:G:145:LYS:N | 4:G:165:GLU:O | 2.49 | 0.41 |
| 10:GA:286:VAL:H | 14:YE:215[C]:GLU:CD | 2.24 | 0.41 |
| 11:GB:9:ILE:HG12 | 11:GB:10:GLU:O | 2.21 | 0.41 |
| 1:GD:243:ILE:HG22 | 1:GD:258:GLY:HA3 | 2.03 | 0.41 |
| 1:GE:382:LEU:HD12 | 1:GE:647:ARG:HH12 | 1.85 | 0.41 |
| 2:GF:103:PHE:CZ | 2:GF:627:GLU:HA | 2.56 | 0.41 |
| 2:GF:784:GLN:HG2 | 2:GF:830:ARG:CB | 2.50 | 0.41 |
| 2:GF:1019:PRO:HG3 | 3:GG:93:ARG:HD3 | 2.02 | 0.41 |
| 1:B:656:GLU:OE2 | 3:GH:265:GLY:HA3 | 2.20 | 0.41 |
| 4:GI:100:ARG:NH2 | 4:GI:128:ASP:OD1 | 2.53 | 0.41 |
| 4:H:65:GLY:HA3 | 4:H:84:ARG:NH1 | 2.36 | 0.41 |
| 5:HB:139:ALA:C | 5:HB:141:GLY:H | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:272:SER:OG | 6:HE:106:THR:N | 2.53 | 0.41 |
| 5:HC:229:ASN:OD1 | 5:HC:230:ILE:N | 2.54 | 0.41 |
| 5:HC:257:SER:O | 5:HC:258:TYR:HB3 | 2.20 | 0.41 |
| 5:HB:590:GLN:O | 5:HC:521:GLY:HA3 | 2.20 | 0.41 |
| 5:HB:569:TYR:N | 5:HC:550:VAL:HB | 2.34 | 0.41 |
| 5:HD:390:LEU:HD23 | 5:HD:391:GLY:N | 2.36 | 0.41 |
| 5:HD:507:ASP:OD1 | 5:HD:510:GLY:N | 2.53 | 0.41 |
| 6:HF:90:PHE:CD2 | 6:HF:126:VAL:HG22 | 2.45 | 0.41 |
| 6:HF:79:PRO:HD2 | 6:HF:193:TRP:CB | 2.51 | 0.41 |
| 6:HG:79:PRO:HD2 | 6:HG:193:TRP:CB | 2.51 | 0.41 |
| 7:HH:212:PRO:HA | 7:HH:215:PHE:HB3 | 2.02 | 0.41 |
| 5:CH:362:GLU:CD | 7:HH:473:LYS:HE2 | 2.40 | 0.41 |
| 7:HH:227:VAL:HG23 | 7:HI:225:LYS:HB3 | 2.03 | 0.41 |
| 7:HI:250:LEU:HD23 | 7:HJ:253:ARG:HH11 | 1.86 | 0.41 |
| 7:HI:262:VAL:CG2 | 7:HJ:260:ARG:HB3 | 2.51 | 0.41 |
| 7:HI:372:CYS:SG | 7:HI:525:VAL:HB | 2.60 | 0.41 |
| 7:HI:476:ASP:OD2 | 7:HJ:454:HIS:HE1 | 2.03 | 0.41 |
| 7:HJ:453:GLU:HG3 | 7:HJ:475:LEU:HD21 | 2.02 | 0.41 |
| 5:I:204:ASP:OD1 | 5:I:205:VAL:N | 2.50 | 0.41 |
| 5:I:326:MET:HE3 | 5:I:326:MET:HB2 | 1.80 | 0.41 |
| 5:I:542:LEU:HD21 | 5:J:569:TYR:CZ | 2.56 | 0.41 |
| 5:I:98:VAL:HG22 | 5:K:90:ASN:HA | 2.03 | 0.41 |
| 8:IB:91:ILE:HG22 | 8:IB:107:TYR:HB3 | 2.02 | 0.41 |
| 9:IC:62:PHE:HZ | 9:IC:127:ALA:HA | 1.86 | 0.41 |
| 5:J:303:PRO:HD2 | 5:J:365:ILE:HD13 | 2.02 | 0.41 |
| 5:K:304:ILE:HG21 | 5:K:309:LEU:HG | 2.02 | 0.41 |
| 6:M:79:PRO:HD2 | 6:M:193:TRP:CB | 2.51 | 0.41 |
| 6:M:195:LEU:HA | 6:M:215:PHE:HD1 | 1.85 | 0.41 |
| 7:O:232:THR:HG23 | 7:O:235:GLU:H | 1.85 | 0.41 |
| 7:O:453:GLU:OE2 | 7:O:471:THR:N | 2.32 | 0.41 |
| 7:P:343:VAL:HG13 | 7:P:524:LYS:O | 2.20 | 0.41 |
| 7:P:99:ARG:HH11 | 7:P:111:ASN:ND2 | 2.17 | 0.41 |
| 7:Q:99:ARG:O | 7:Q:114:SER:HA | 2.21 | 0.41 |
| 7:Q:233:GLN:OE1 | 7:Q:252:GLY:HA3 | 2.21 | 0.41 |
| 7:P:262:VAL:CG2 | 7:Q:260:ARG:HB3 | 2.51 | 0.41 |
| 10:U:139:SER:HA | 10:U:203:ARG:HG2 | 2.01 | 0.41 |
| 11:V:36:PHE:CD1 | 11:V:180:PHE:HZ | 2.39 | 0.41 |
| 12:W:30:PRO:HG2 | 12:W:177:TRP:HE1 | 1.86 | 0.41 |
| 1:X:390:GLU:O | 1:X:394:ASN:ND2 | 2.53 | 0.41 |
| 1:X:413:TYR:HB2 | 1:X:639:LEU:O | 2.21 | 0.41 |
| 1:Y:596:ASN:OD1 | 1:Y:596:ASN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:187[B]:ARG:HD3 | 13:YA:187[B]:ARG:HA | 1.86 | 0.41 |
| 13:YA:239[F]:GLU:H | 13:YA:239[F]:GLU:CD | 2.24 | 0.41 |
| 13:YA:296[F]:LEU:HA | 13:YA:296[F]:LEU:HD12 | 1.84 | 0.41 |
| 13:YA:72[B]:SER:O | 13:YC:61[B]:ILE:HD11 | 2.20 | 0.41 |
| 13:YB:224[A]:GLN:H | 13:YB:224[A]:GLN:HG3 | 1.65 | 0.41 |
| 13:YB:239[B]:GLU:CD | 13:YB:239[B]:GLU:H | 2.24 | 0.41 |
| 13:YB:293[C]:ASN:HA | 13:YB:296[C]:LEU:HB2 | 2.02 | 0.41 |
| 13:YB:410[B]:GLU:O | 13:YB:426[B]:PRO:HA | 2.21 | 0.41 |
| 13:YB:399[B]:HIS:ND1 | 13:YB:417[B]:PRO:HD3 | 2.36 | 0.41 |
| 13:YB:410[E]:GLU:O | 13:YB:426[E]:PRO:HA | 2.21 | 0.41 |
| 13:YB:506[F]:VAL:HG21 | 13:YC:502[F]:VAL:HG21 | 2.02 | 0.41 |
| 13:YB:558[C]:SER:O | 13:YC:551[C]:THR:HA | 2.21 | 0.41 |
| 13:YC:239[C]:GLU:H | 13:YC:239[C]:GLU:CD | 2.24 | 0.41 |
| 13:YC:239[F]:GLU:CD | 13:YC:239[F]:GLU:H | 2.24 | 0.41 |
| 13:YC:252[B]:MET:HE3 | 13:YC:252[B]:MET:HB3 | 1.81 | 0.41 |
| 13:YC:280[C]:MET:O | 13:YC:284[C]:MET:HG2 | 2.20 | 0.41 |
| 13:YC:47[E]:ILE:HG23 | 14:YF:123[E]:PRO:CG | 2.49 | 0.41 |
| 13:YB:506[F]:VAL:HA | 13:YC:498[F]:VAL:O | 2.20 | 0.41 |
| 14:YD:51[A]:MET:SD | 14:YD:108[A]:GLU:HA | 2.61 | 0.41 |
| 14:YD:115[B]:ILE:O | 14:YF:243[B]:HIS:HD2 | 2.04 | 0.41 |
| 14:YD:124[A]:PHE:CZ | 14:YD:135[A]:MET:HG2 | 2.56 | 0.41 |
| 14:YD:210[B]:PRO:HB2 | 14:YD:228[B]:TYR:CD2 | 2.56 | 0.41 |
| 14:YD:279[C]:ARG:HD3 | 14:YD:279[C]:ARG:HA | 1.43 | 0.41 |
| 14:YD:290[B]:ASN:O | 14:YD:292[B]:TYR:N | 2.54 | 0.41 |
| 14:YD:345[B]:GLU:HB3 | 14:YD:352[B]:VAL:HG13 | 2.03 | 0.41 |
| 14:YD:345[E]:GLU:HB3 | 14:YD:352[E]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:124[F]:PHE:CZ | 14:YE:135[F]:MET:HG2 | 2.56 | 0.41 |
| 14:YE:212[C]:ILE:HG12 | 14:YE:228[C]:TYR:HB2 | 2.03 | 0.41 |
| 14:YE:259[E]:LEU:HA | 14:YE:259[E]:LEU:HD23 | 1.83 | 0.41 |
| 14:YE:238[D]:THR:N | 14:YE:307[D]:TYR:O | 2.53 | 0.41 |
| 11:GB:182:ASN:ND2 | 14:YE:327[C]:ASN:HD22 | 2.18 | 0.41 |
| 14:YE:51[F]:MET:SD | 14:YE:108[F]:GLU:HA | 2.61 | 0.41 |
| 14:YF:51[C]:MET:SD | 14:YF:108[C]:GLU:HA | 2.61 | 0.41 |
| 14:YF:51[F]:MET:SD | 14:YF:108[F]:GLU:HA | 2.61 | 0.41 |
| 14:YF:10[F]:PRO:HB2 | 14:YF:74[F]:VAL:HG21 | 2.03 | 0.41 |
| 14:YF:124[A]:PHE:CZ | 14:YF:135[A]:MET:HG2 | 2.56 | 0.41 |
| 14:YF:43[B]:SER:O | 14:YF:189[B]:TRP:HB2 | 2.20 | 0.41 |
| 11:V:190:LYS:NZ | 14:YF:24[D]:SER:HA | 2.34 | 0.41 |
| 14:YF:238[A]:THR:N | 14:YF:307[A]:TYR:O | 2.53 | 0.41 |
| 14:YF:345[E]:GLU:HB3 | 14:YF:352[E]:VAL:HG13 | 2.03 | 0.41 |
| 2:Z:306:ARG:C | 2:Z:307:ILE:HD12 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:380:ILE:HB | 2:Z:396:ILE:HG21 | 2.01 | 0.41 |
| 2:Z:412:THR:OG1 | 2:Z:413:TRP:N | 2.53 | 0.41 |
| 2:Z:431:TYR:HB3 | 2:Z:485:TYR:OH | 2.20 | 0.41 |
| 2:Z:740:ILE:O | 2:Z:743:SER:HB3 | 2.20 | 0.41 |
| 2:Z:884:HIS:CG | 2:Z:885:PRO:HD2 | 2.56 | 0.41 |
| 2:Z:899:PHE:O | 2:Z:900:ILE:HD13 | 2.21 | 0.41 |
| 2:Z:976:SER:C | 2:Z:977:ILE:HG13 | 2.40 | 0.41 |
| 15:ZA:56[A]:HIS:CD2 | 15:ZA:83[A]:CYS:HB2 | 2.56 | 0.41 |
| 1:A:433:GLU:OE2 | 1:A:655:LEU:HD11 | 2.20 | 0.41 |
| 1:A:485:VAL:HG22 | 1:A:624:TYR:CD1 | 2.53 | 0.41 |
| 5:AC:151:ILE:O | 5:AC:152:ASP:HB3 | 2.21 | 0.41 |
| 5:AC:162:VAL:HA | 5:AC:246:THR:O | 2.20 | 0.41 |
| 5:AC:486:VAL:HG11 | 5:AE:590:GLN:NE2 | 2.36 | 0.41 |
| 5:AD:139:ALA:HB3 | 5:AD:140:PRO:HD3 | 2.01 | 0.41 |
| 5:AD:150:GLN:C | 5:AD:151:ILE:HG13 | 2.40 | 0.41 |
| 5:AE:150:GLN:HG3 | 5:AE:152:ASP:HB3 | 2.01 | 0.41 |
| 5:AE:340:VAL:HG21 | 6:AF:174:TYR:H | 1.86 | 0.41 |
| 5:AD:460:TYR:CE1 | 5:AE:458:THR:HG23 | 2.55 | 0.41 |
| 6:AF:82:VAL:HG23 | 6:AF:187:LYS:HE3 | 2.01 | 0.41 |
| 6:AG:70:ILE:HD12 | 6:AG:196:LEU:HD11 | 2.03 | 0.41 |
| 7:AI:134:SER:H | 7:AI:142:ILE:CD1 | 2.33 | 0.41 |
| 7:AI:77:THR:CG2 | 7:AI:80:THR:H | 2.33 | 0.41 |
| 7:AI:44:VAL:HG21 | 7:AJ:25:PHE:HB3 | 2.03 | 0.41 |
| 7:AJ:262:VAL:CG2 | 7:BA:260:ARG:HB3 | 2.51 | 0.41 |
| 1:B:92:ALA:O | 1:B:95:ASP:N | 2.54 | 0.41 |
| 7:AJ:476:ASP:OD2 | 7:BA:454:HIS:HE1 | 2.03 | 0.41 |
| 7:BA:4:ASN:O | 7:BA:8:HIS:N | 2.48 | 0.41 |
| 8:BB:91:ILE:HG22 | 8:BB:107:TYR:HB3 | 2.02 | 0.41 |
| 11:BF:36:PHE:CD1 | 11:BF:180:PHE:HZ | 2.39 | 0.41 |
| 1:BH:414:LEU:HD23 | 1:BH:486:ARG:HE | 1.84 | 0.41 |
| 1:BH:572:TYR:CE2 | 1:BH:574:GLY:HA3 | 2.56 | 0.41 |
| 1:BH:580:LEU:C | 1:BH:580:LEU:HD12 | 2.41 | 0.41 |
| 2:BJ:577:GLY:N | 2:BJ:606:ASP:O | 2.54 | 0.41 |
| 2:BJ:644:ASP:HB2 | 2:BJ:646:ARG:HG2 | 2.01 | 0.41 |
| 2:BJ:752:TYR:O | 2:BJ:753:ASN:OD1 | 2.39 | 0.41 |
| 2:C:484:HIS:O | 2:C:485:TYR:HB3 | 2.21 | 0.41 |
| 2:C:912:ILE:HD11 | 3:D:329:ASN:HB2 | 2.03 | 0.41 |
| 2:BJ:947:VAL:HB | 3:CA:119:TYR:HB3 | 2.03 | 0.41 |
| 4:CC:44:ASP:O | 4:CC:59:GLN:NE2 | 2.52 | 0.41 |
| 5:CF:326:MET:HG3 | 5:CF:327:PRO:CD | 2.43 | 0.41 |
| 5:CF:590:GLN:O | 5:CG:521:GLY:HA3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CG:139:ALA:HB3 | 5:CG:140:PRO:HD3 | 2.01 | 0.41 |
| 5:CG:56:SER:OG | 5:CG:57:GLY:N | 2.53 | 0.41 |
| 5:CH:258:TYR:HD1 | 5:CH:386:PHE:HD1 | 1.67 | 0.41 |
| 5:CH:399:ILE:O | 5:CH:402:GLU:HB3 | 2.21 | 0.41 |
| 5:CH:497:PRO:HG2 | 5:CH:498:ASN:ND2 | 2.35 | 0.41 |
| 5:CH:264:ARG:HH12 | 6:CI:2:SER:N | 2.18 | 0.41 |
| 6:CJ:70:ILE:HD12 | 6:CJ:196:LEU:HD11 | 2.03 | 0.41 |
| 6:DA:88:TRP:HB3 | 6:DA:90:PHE:CE1 | 2.55 | 0.41 |
| 7:DC:335:ASN:OD1 | 7:DC:336:GLU:N | 2.53 | 0.41 |
| 7:DB:515:TRP:CH2 | 7:DC:439:ILE:HG12 | 2.56 | 0.41 |
| 7:DB:479:ASN:OD1 | 7:DC:454:HIS:ND1 | 2.53 | 0.41 |
| 7:DB:425:LEU:HD11 | 7:DC:505:PRO:O | 2.19 | 0.41 |
| 7:DB:98:THR:OG1 | 7:DD:100:TYR:OH | 1.91 | 0.41 |
| 7:DD:73:THR:HG23 | 7:DD:74:LYS:N | 2.36 | 0.41 |
| 7:DD:99:ARG:O | 7:DD:114:SER:HA | 2.21 | 0.41 |
| 8:DF:91:ILE:HG22 | 8:DF:107:TYR:HB3 | 2.02 | 0.41 |
| 9:DG:85:GLU:OE2 | 9:DG:87:ARG:NH2 | 2.53 | 0.41 |
| 3:E:191:LEU:HD23 | 3:E:191:LEU:HA | 1.76 | 0.41 |
| 1:EB:448:TYR:HA | 1:EB:452:VAL:CG1 | 2.49 | 0.41 |
| 1:EB:494:THR:HG22 | 1:EB:498:GLY:HA2 | 2.03 | 0.41 |
| 1:EB:565:GLU:OE1 | 1:EB:571:PRO:HD3 | 2.20 | 0.41 |
| 1:EB:62:TYR:CZ | 1:EB:66:TYR:HE2 | 2.38 | 0.41 |
| 1:EB:66:TYR:O | 1:EB:69:GLN:N | 2.54 | 0.41 |
| 2:EC:1005:ARG:NH1 | 5:EI:12:ASP:OD2 | 2.53 | 0.41 |
| 3:ED:197:ASP:N | 3:ED:197:ASP:OD1 | 2.54 | 0.41 |
| 4:EG:216:THR:CG2 | 4:EH:222:LEU:HD13 | 2.51 | 0.41 |
| 5:EI:162:VAL:HA | 5:EI:246:THR:O | 2.20 | 0.41 |
| 5:EI:348:THR:H | 7:HH:233:GLN:HG3 | 1.84 | 0.41 |
| 5:EI:322:GLY:N | 5:EI:360:THR:HG23 | 2.35 | 0.41 |
| 6:FC:145:SER:O | 6:FC:159:THR:N | 2.45 | 0.41 |
| 6:FC:42:GLN:N | 6:FC:42:GLN:OE1 | 2.52 | 0.41 |
| 7:FE:127:ASN:O | 7:FE:131:THR:HG23 | 2.20 | 0.41 |
| 7:FF:212:PRO:HG3 | 7:FG:199:VAL:HG12 | 2.03 | 0.41 |
| 7:FE:439:ILE:HG12 | 7:FG:515:TRP:CZ3 | 2.56 | 0.41 |
| 7:FF:59:PHE:CZ | 7:FG:55:LYS:HG3 | 2.56 | 0.41 |
| 8:FH:49:ILE:HG23 | 8:FH:60:VAL:O | 2.21 | 0.41 |
| 9:FJ:10:ASP:O | 9:FJ:26:SER:N | 2.48 | 0.41 |
| 10:GA:133:LYS:HB3 | 10:GA:208:THR:O | 2.19 | 0.41 |
| 11:GB:133:TRP:CE2 | 11:GB:150:LEU:HD11 | 2.55 | 0.41 |
| 12:GC:124:MET:HG3 | 12:GC:170:ASN:ND2 | 2.35 | 0.41 |
| 12:GC:215:MET:CE | 12:IF:99:SER:HB2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:433:GLU:OE2 | 1:GD:655:LEU:HD11 | 2.20 | 0.41 |
| 1:GD:418:THR:HG22 | 1:GD:482:ILE:HG22 | 2.02 | 0.41 |
| 1:GE:190:LYS:O | 1:GE:191:ASN:HB2 | 2.20 | 0.41 |
| 2:GF:793:CYS:HB3 | 2:GF:813:ILE:HG21 | 2.03 | 0.41 |
| 2:GF:821:ILE:HD12 | 2:GF:821:ILE:H | 1.85 | 0.41 |
| 2:GF:821:ILE:N | 2:GF:824:GLN:NE2 | 2.69 | 0.41 |
| 2:GF:884:HIS:CG | 2:GF:885:PRO:HD2 | 2.56 | 0.41 |
| 3:GH:210:VAL:HG13 | 3:GH:211:PRO:HD2 | 2.02 | 0.41 |
| 2:EC:509:TYR:CD2 | 3:GH:229:LEU:HD23 | 2.56 | 0.41 |
| 4:GJ:17:ASN:OD1 | 4:GJ:18:ALA:N | 2.53 | 0.41 |
| 4:GJ:167:MET:O | 4:HA:163:SER:HB3 | 2.21 | 0.41 |
| 4:HA:65:GLY:HA3 | 4:HA:84:ARG:NH1 | 2.36 | 0.41 |
| 5:HB:162:VAL:HA | 5:HB:246:THR:O | 2.20 | 0.41 |
| 5:HB:271:THR:HB | 5:HB:273:LYS:HG2 | 2.03 | 0.41 |
| 5:HB:318:GLN:HB3 | 6:HG:4:LEU:HD12 | 2.02 | 0.41 |
| 5:HB:81:LEU:HD22 | 5:HB:143:TRP:CZ3 | 2.56 | 0.41 |
| 5:HB:90:ASN:OD1 | 5:HC:49:TRP:HB2 | 2.21 | 0.41 |
| 5:HC:559:PRO:HA | 5:HC:561:GLU:OE2 | 2.21 | 0.41 |
| 5:HC:326:MET:CE | 5:HD:264:ARG:HB3 | 2.51 | 0.41 |
| 5:HB:549:SER:N | 5:HD:569:TYR:O | 2.54 | 0.41 |
| 7:HH:127:ASN:O | 7:HH:131:THR:HG23 | 2.20 | 0.41 |
| 7:HH:134:SER:H | 7:HH:142:ILE:CD1 | 2.33 | 0.41 |
| 7:HH:228:ILE:O | 7:HI:225:LYS:HA | 2.20 | 0.41 |
| 7:HI:196:VAL:HA | 7:HI:199:VAL:HG22 | 2.03 | 0.41 |
| 6:FB:218:THR:CB | 7:HI:205:ARG:HH12 | 2.31 | 0.41 |
| 7:HI:433:TYR:CE2 | 7:HI:436:GLU:HB2 | 2.56 | 0.41 |
| 7:HJ:73:THR:HG23 | 7:HJ:74:LYS:N | 2.36 | 0.41 |
| 7:HJ:77:THR:OG1 | 7:HJ:78:PRO:HD2 | 2.20 | 0.41 |
| 5:I:133:LEU:HA | 5:I:133:LEU:HD23 | 1.81 | 0.41 |
| 5:I:352:SER:HB2 | 5:I:354:THR:O | 2.21 | 0.41 |
| 8:IA:118:ARG:NH2 | 8:IB:62:GLY:O | 2.54 | 0.41 |
| 8:IA:49:ILE:HG23 | 8:IA:60:VAL:O | 2.21 | 0.41 |
| 12:IF:96:THR:OG1 | 12:IF:104:PHE:O | 2.31 | 0.41 |
| 12:IF:113:PHE:CE1 | 12:IF:170:ASN:HA | 2.56 | 0.41 |
| 12:IF:196:GLU:HG2 | 12:IF:218:MET:O | 2.21 | 0.41 |
| 5:J:94:ARG:CD | 5:J:134:GLU:HG2 | 2.51 | 0.41 |
| 5:J:323:THR:HG21 | 5:J:354:THR:HG23 | 2.02 | 0.41 |
| 5:J:338:ASP:HB3 | 5:J:349:TRP:CD1 | 2.56 | 0.41 |
| 5:K:104:VAL:HG22 | 5:K:105:ASN:N | 2.35 | 0.41 |
| 5:J:70:ILE:HG13 | 5:K:212:PHE:CD1 | 55.00 | 0.41 |
| 5:K:304:ILE:HD12 | 5:K:306:PRO:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:M:10:VAL:HA | 6:N:13:ARG:CD | 2.33 | 0.41 |
| 6:M:117:THR:H | 6:M:120:MET:HE3 | 1.86 | 0.41 |
| 6:L:19:GLY:H | 6:M:13:ARG:CZ | 2.33 | 0.41 |
| 6:N:82:VAL:HG23 | 6:N:187:LYS:HE3 | 2.01 | 0.41 |
| 7:O:185:GLU:HA | 7:Q:193:LEU:HB2 | 2.02 | 0.41 |
| 7:P:17:LYS:HD2 | 7:P:18:PHE:H | 1.86 | 0.41 |
| 7:Q:232:THR:HG23 | 7:Q:235:GLU:H | 1.85 | 0.41 |
| 7:Q:351:ALA:O | 7:Q:520:ASN:ND2 | 2.54 | 0.41 |
| 10:U:221:ALA:O | 10:U:225:ILE:N | 2.46 | 0.41 |
| 11:V:133:TRP:CE2 | 11:V:150:LEU:HD11 | 2.55 | 0.41 |
| 11:V:88:THR:O | 11:V:163:ASN:ND2 | 2.53 | 0.41 |
| 1:X:337:GLN:O | 1:X:348:PHE:HZ | 2.02 | 0.41 |
| 1:Y:322:ILE:O | 1:Y:325:ILE:HB | 2.21 | 0.41 |
| 13:YA:239[E]:GLU:CD | 13:YA:239[E]:GLU:H | 2.24 | 0.41 |
| 13:YA:239[D]:GLU:CD | 13:YA:239[D]:GLU:H | 2.24 | 0.41 |
| 13:YA:293[C]:ASN:HA | 13:YA:296[C]:LEU:HB2 | 2.02 | 0.41 |
| 13:YA:410[B]:GLU:O | 13:YA:426[B]:PRO:HA | 2.21 | 0.41 |
| 13:YA:410[C]:GLU:O | 13:YA:426[C]:PRO:HA | 2.20 | 0.41 |
| 13:YA:463[A]:ILE:HA | 13:YC:471[A]:LEU:O | 2.20 | 0.41 |
| 13:YA:486[A]:GLU:CB | 13:YC:490[A]:VAL:HG11 | 2.50 | 0.41 |
| 13:YA:486[C]:GLU:CB | 13:YC:490[C]:VAL:HG11 | 2.51 | 0.41 |
| 13:YA:552[F]:GLU:HB2 | 13:YB:544[F]:TRP:HB2 | 2.03 | 0.41 |
| 13:YA:66[A]:MET:HA | 13:YA:66[A]:MET:HE3 | 2.02 | 0.41 |
| 13:YA:75[B]:GLY:HA2 | 13:YC:61[B]:ILE:HB | 2.02 | 0.41 |
| 13:YB:187[B]:ARG:HD3 | 13:YB:187[B]:ARG:HA | 1.86 | 0.41 |
| 13:YB:24[F]:LEU:HD23 | 14:YE:259[F]:LEU:CD2 | 2.49 | 0.41 |
| 13:YB:293[F]:ASN:HA | 13:YB:296[F]:LEU:HB2 | 2.02 | 0.41 |
| 13:YB:410[A]:GLU:O | 13:YB:426[A]:PRO:HA | 2.20 | 0.41 |
| 13:YB:436[E]:ASP:HB3 | 13:YC:429[E]:ARG:HA | 2.03 | 0.41 |
| 13:YB:566[B]:THR:HG23 | 13:YC:558[B]:SER:HA | 2.01 | 0.41 |
| 13:YC:24[E]:LEU:HD12 | 13:YC:24[E]:LEU:HA | 1.63 | 0.41 |
| 13:YB:436[A]:ASP:HB3 | 13:YC:429[A]:ARG:HA | 2.02 | 0.41 |
| 13:YA:445[B]:ASP:HA | 13:YC:453[B]:ASP:O | 2.20 | 0.41 |
| 13:YA:445[C]:ASP:HA | 13:YC:453[C]:ASP:O | 2.20 | 0.41 |
| 13:YA:486[E]:GLU:CB | 13:YC:490[E]:VAL:HG11 | 2.51 | 0.41 |
| 13:YB:558[A]:SER:O | 13:YC:551[A]:THR:HA | 2.21 | 0.41 |
| 13:YB:558[B]:SER:O | 13:YC:551[B]:THR:HA | 2.21 | 0.41 |
| 13:YA:550[F]:TRP:HB2 | 13:YC:554[F]:MET:HG3 | 2.02 | 0.41 |
| 13:YA:558[A]:SER:HA | 13:YC:566[A]:THR:HG23 | 2.01 | 0.41 |
| 14:YD:136[B]:LEU:HD21 | 14:YD:166[B]:PHE:CE2 | 2.56 | 0.41 |
| 14:YD:174[B]:ARG:CG | 14:YD:188[B]:VAL:HG22 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YD:172[C]:TYR:CZ | 14:YD:176[C]:VAL:HG21 | 2.55 | 0.41 |
| 14:YD:209[F]:TYR:HB3 | 14:YD:324[F]:ILE:HG12 | 2.03 | 0.41 |
| 14:YD:259[C]:LEU:HA | 14:YD:259[C]:LEU:HD23 | 1.82 | 0.41 |
| 14:YD:45[C]:TYR:HD1 | 14:YD:45[C]:TYR:HA | 1.69 | 0.41 |
| 14:YD:47[F]:ARG:NH1 | 14:YD:341[F]:GLU:OE1 | 2.54 | 0.41 |
| 14:YD:10[F]:PRO:HB2 | 14:YD:74[F]:VAL:HG21 | 2.03 | 0.41 |
| 14:YE:136[A]:LEU:HD21 | 14:YE:166[A]:PHE:CE2 | 2.56 | 0.41 |
| 14:YE:174[E]:ARG:CG | 14:YE:188[E]:VAL:HG22 | 2.51 | 0.41 |
| 14:YE:210[B]:PRO:HB2 | 14:YE:228[B]:TYR:CD2 | 2.56 | 0.41 |
| 13:YB:24[C]:LEU:HD23 | 14:YE:259[C]:LEU:CD2 | 2.50 | 0.41 |
| 14:YE:259[A]:LEU:HD23 | 14:YE:259[A]:LEU:HA | 1.83 | 0.41 |
| 14:YE:355[A]:LEU:HA | 14:YE:355[A]:LEU:HD23 | 1.87 | 0.41 |
| 14:YF:51[A]:MET:SD | 14:YF:108[A]:GLU:HA | 2.61 | 0.41 |
| 14:YF:114[F]:SER:HA | 14:YF:167[F]:GLU:OE1 | 2.19 | 0.41 |
| 14:YF:174[C]:ARG:CG | 14:YF:188[C]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:174[D]:ARG:CG | 14:YF:188[D]:VAL:HG22 | 2.51 | 0.41 |
| 14:YF:290[C]:ASN:O | 14:YF:292[C]:TYR:N | 2.54 | 0.41 |
| 14:YF:290[D]:ASN:O | 14:YF:292[D]:TYR:N | 2.54 | 0.41 |
| 14:YF:16[A]:LEU:CD2 | 14:YF:29[A]:VAL:HB | 2.51 | 0.41 |
| 14:YF:355[E]:LEU:HD23 | 14:YF:355[E]:LEU:HA | 1.87 | 0.41 |
| 14:YF:45[E]:TYR:HD1 | 14:YF:45[E]:TYR:HA | 1.69 | 0.41 |
| 14:YF:75[F]:ALA:HB2 | 14:YF:83[F]:VAL:HA | 2.01 | 0.41 |
| 2:Z:217:GLN:HG2 | 2:Z:218:THR:N | 2.36 | 0.41 |
| 2:Z:883:VAL:HG13 | 2:Z:884:HIS:N | 2.36 | 0.41 |
| 1:A:243:ILE:HG22 | 1:A:258:GLY:HA3 | 2.03 | 0.41 |
| 1:A:448:TYR:CE2 | 1:A:642:PHE:HB2 | 2.55 | 0.41 |
| 1:A:55:VAL:O | 1:A:58:ASP:HB3 | 2.20 | 0.41 |
| 1:A:413:TYR:HB2 | 1:A:639:LEU:O | 2.21 | 0.41 |
| 5:AC:128:VAL:HB | 5:AC:131:SER:OG | 2.21 | 0.41 |
| 5:AC:137:TYR:HA | 5:AC:143:TRP:CD1 | 2.55 | 0.41 |
| 5:AC:153:LYS:HG2 | 5:AC:154:ILE:N | 2.36 | 0.41 |
| 5:AC:352:SER:HB2 | 5:AC:354:THR:O | 2.21 | 0.41 |
| 5:AD:147:LYS:HG2 | 5:AE:154:ILE:O | 2.21 | 0.41 |
| 5:AD:255:ARG:HH21 | 5:AE:249:ASP:HB2 | 1.85 | 0.41 |
| 5:AE:192:ARG:HB2 | 5:AE:245:GLU:H | 1.85 | 0.41 |
| 5:AD:11:VAL:HG22 | 5:AE:20:ARG:NE | 2.35 | 0.41 |
| 5:AE:304:ILE:HG21 | 5:AE:309:LEU:HG | 2.02 | 0.41 |
| 5:AE:433:VAL:HG12 | 5:AE:434:GLU:N | 2.36 | 0.41 |
| 5:AE:507:ASP:OD1 | 5:AE:510:GLY:N | 2.53 | 0.41 |
| 6:AF:71:ILE:O | 6:AF:215:PHE:N | 2.36 | 0.41 |
| 6:AH:82:VAL:HG23 | 6:AH:187:LYS:HE3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AI:375:TYR:CE2 | 7:AI:390:PRO:HB2 | 2.53 | 0.41 |
| 7:AJ:17:LYS:HD2 | 7:AJ:18:PHE:H | 1.86 | 0.41 |
| 7:AJ:372:CYS:SG | 7:AJ:525:VAL:HB | 2.60 | 0.41 |
| 7:AJ:458:GLY:O | 7:AJ:461:GLY:N | 2.41 | 0.41 |
| 1:B:352:ARG:O | 1:B:353:PHE:HB2 | 2.21 | 0.41 |
| 1:B:382:LEU:HA | 1:B:382:LEU:HD23 | 1.78 | 0.41 |
| 1:B:448:TYR:HA | 1:B:452:VAL:CG1 | 2.49 | 0.41 |
| 7:BA:134:SER:N | 7:BA:142:ILE:HD11 | 2.35 | 0.41 |
| 7:BA:73:THR:HG23 | 7:BA:74:LYS:N | 2.36 | 0.41 |
| 8:BC:98:GLU:N | 8:BC:98:GLU:OE1 | 2.48 | 0.41 |
| 10:BE:213:PRO:HG3 | 10:BE:219:LEU:HD12 | 2.03 | 0.41 |
| 1:BI:22:VAL:HG12 | 1:BI:23:GLY:N | 2.36 | 0.41 |
| 1:BI:394:ASN:O | 1:BI:397:LYS:HG2 | 2.21 | 0.41 |
| 2:BJ:307:ILE:HG22 | 2:BJ:308:ALA:N | 2.36 | 0.41 |
| 2:BJ:315:ASP:O | 2:BJ:316:ASP:HB2 | 2.20 | 0.41 |
| 2:BJ:411:LYS:O | 2:BJ:412:THR:HB | 2.21 | 0.41 |
| 2:BJ:417:PHE:CE1 | 2:BJ:423:GLU:HG2 | 2.56 | 0.41 |
| 2:BJ:528:ASN:HD21 | 3:ED:285:PRO:HB2 | 1.85 | 0.41 |
| 2:BJ:729:SER:OG | 2:BJ:730:ARG:N | 2.54 | 0.41 |
| 2:BJ:788:THR:OG1 | 2:BJ:789:ALA:N | 2.54 | 0.41 |
| 2:C:253:ILE:HG13 | 2:C:300:LEU:CD2 | 2.51 | 0.41 |
| 2:C:29:GLY:HA2 | 3:E:60:TYR:HB3 | 2.03 | 0.41 |
| 2:C:341:LEU:HD23 | 2:C:341:LEU:HA | 1.84 | 0.41 |
| 2:C:600:PHE:CE2 | 2:C:604:VAL:HB | 2.56 | 0.41 |
| 2:C:613:LYS:HB3 | 1:Y:619:GLN:HE22 | 1.86 | 0.41 |
| 2:C:103:PHE:CZ | 2:C:627:GLU:HA | 2.56 | 0.41 |
| 3:CA:132:ARG:NH1 | 3:CA:189:GLU:OE2 | 2.49 | 0.41 |
| 4:CC:201:LYS:NZ | 4:CC:220:ASN:OD1 | 2.37 | 0.41 |
| 5:CF:103:ASN:CG | 5:CF:104:VAL:H | 2.24 | 0.41 |
| 5:CF:104:VAL:HG22 | 5:CF:105:ASN:H | 1.86 | 0.41 |
| 5:CF:544:VAL:HA | 5:CH:569:TYR:CE1 | 2.56 | 0.41 |
| 5:CG:180:VAL:HG22 | 5:CG:181:PHE:H | 1.84 | 0.41 |
| 5:CF:319:GLU:HG3 | 5:CG:262:GLN:OE1 | 2.20 | 0.41 |
| 5:CG:98:VAL:HG12 | 5:CG:99:PHE:CD2 | 2.46 | 0.41 |
| 5:CH:89:TYR:CE1 | 5:CH:137:TYR:CZ | 3.09 | 0.41 |
| 6:CI:88:TRP:HB3 | 6:CI:90:PHE:CE1 | 2.55 | 0.41 |
| 3:D:47:TRP:HH2 | 3:D:58:PRO:HB3 | 1.82 | 0.41 |
| 7:DB:134:SER:H | 7:DB:142:ILE:CD1 | 2.33 | 0.41 |
| 7:DB:325:TYR:CD1 | 7:DB:330:ARG:HA | 2.55 | 0.41 |
| 7:DB:443:SER:HA | 7:DD:509:GLY:O | 2.20 | 0.41 |
| 7:DC:146:SER:HA | 7:DC:164:LYS:HZ2 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:474:GLY:HA2 | 7:DC:472:ARG:CZ | 2.51 | 0.41 |
| 7:DC:397:GLY:N | 7:DD:402:GLY:O | 2.50 | 0.41 |
| 7:DB:503:ASN:ND2 | 7:DD:446:LYS:H | 2.19 | 0.41 |
| 8:DE:89:GLN:HB3 | 8:DE:134:PRO:CG | 2.50 | 0.41 |
| 10:DH:139:SER:HA | 10:DH:203:ARG:HG2 | 2.01 | 0.41 |
| 12:DJ:124:MET:HG3 | 12:DJ:170:ASN:ND2 | 2.35 | 0.41 |
| 3:E:115:ASN:HA | 3:E:121:ALA:HA | 2.02 | 0.41 |
| 3:E:134:LEU:HA | 3:E:134:LEU:HD23 | 1.72 | 0.41 |
| 1:EA:222:THR:O | 1:EA:223:ILE:HG12 | 2.21 | 0.41 |
| 1:EA:572:TYR:CE2 | 1:EA:574:GLY:HA3 | 2.56 | 0.41 |
| 1:EB:530:LEU:HD12 | 1:EB:532:GLU:H | 1.84 | 0.41 |
| 2:EC:196:GLU:OE1 | 2:EC:196:GLU:N | 2.42 | 0.41 |
| 2:EC:253:ILE:HG13 | 2:EC:300:LEU:CD2 | 2.51 | 0.41 |
| 2:EC:379:ILE:HD11 | 2:EC:402:GLY:H | 1.86 | 0.41 |
| 2:EC:439:LYS:HG3 | 2:EC:440:LEU:HD12 | 2.02 | 0.41 |
| 2:EC:442:SER:HA | 2:EC:491:ILE:HD13 | 2.03 | 0.41 |
| 2:EC:784:GLN:HG2 | 2:EC:830:ARG:CB | 2.50 | 0.41 |
| 2:EC:906:LEU:HD12 | 2:EC:907:LYS:N | 2.35 | 0.41 |
| 3:ED:138:ASP:HA | 3:ED:150:LYS:HE3 | 2.03 | 0.41 |
| 3:ED:310:ILE:HG13 | 3:ED:311:TYR:N | 2.36 | 0.41 |
| 3:ED:79:VAL:HG12 | 3:ED:80:LYS:O | 2.21 | 0.41 |
| 3:EE:134:LEU:HA | 3:EE:134:LEU:HD23 | 1.72 | 0.41 |
| 4:EG:205:THR:HG22 | 4:EH:284:ILE:HD11 | 2.03 | 0.41 |
| 4:EH:65:GLY:HA3 | 4:EH:84:ARG:NH1 | 2.36 | 0.41 |
| 5:EI:486:VAL:HG11 | 5:FA:590:GLN:NE2 | 2.36 | 0.41 |
| 5:EJ:180:VAL:HG22 | 5:EJ:181:PHE:H | 1.84 | 0.41 |
| 5:EJ:397:ASP:OD1 | 5:EJ:398:GLU:HG2 | 2.21 | 0.41 |
| 5:EJ:559:PRO:HA | 5:EJ:561:GLU:OE2 | 2.21 | 0.41 |
| 5:EJ:58:GLN:N | 5:EJ:58:GLN:OE1 | 2.42 | 0.41 |
| 5:FA:177:PHE:O | 5:FA:230:ILE:HG13 | 2.21 | 0.41 |
| 6:FC:100:PRO:O | 6:FC:103:SER:OG | 2.18 | 0.41 |
| 6:FD:126:VAL:HG13 | 6:FD:156:LEU:HD11 | 2.03 | 0.41 |
| 6:FD:12:SER:HG | 6:FD:17:PHE:HD2 | 1.65 | 0.41 |
| 6:FD:96:ASP:OD1 | 6:FD:98:SER:OG | 2.32 | 0.41 |
| 7:FE:171:LYS:HA | 7:FE:174:ALA:HB3 | 2.03 | 0.41 |
| 7:FE:176:ILE:HG12 | 7:FE:177:ALA:N | 2.33 | 0.41 |
| 7:FE:228:ILE:HG21 | 7:FE:244:ALA:HB2 | 2.01 | 0.41 |
| 7:FE:456:ASP:CB | 7:FE:462:ASN:HD21 | 2.34 | 0.41 |
| 7:FE:78:PRO:HB2 | 7:FF:69:GLY:HA2 | 2.03 | 0.41 |
| 7:FE:190:VAL:HB | 7:FF:188:GLN:C | 2.41 | 0.41 |
| 7:FF:283:TRP:CZ3 | 7:FF:284:ASN:HB3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:315:ILE:O | 7:FF:321:MET:HA | 2.21 | 0.41 |
| 7:FF:335:ASN:OD1 | 7:FF:336:GLU:N | 2.53 | 0.41 |
| 7:FF:343:VAL:HG13 | 7:FF:524:LYS:O | 2.21 | 0.41 |
| 7:FE:447:HIS:CE1 | 7:FG:445:HIS:CE1 | 3.08 | 0.41 |
| 7:FG:453:GLU:HG3 | 7:FG:475:LEU:HD21 | 2.02 | 0.41 |
| 4:G:65:GLY:HA3 | 4:G:84:ARG:NH1 | 2.36 | 0.41 |
| 1:GD:23:GLY:HA2 | 1:GD:68:GLN:NE2 | 2.35 | 0.41 |
| 1:GE:148:ARG:HG2 | 1:GE:149:GLU:HG3 | 2.01 | 0.41 |
| 1:GE:244:SER:O | 1:GE:253:THR:OG1 | 2.34 | 0.41 |
| 1:GE:220:THR:HA | 1:GE:260:LEU:HD13 | 2.03 | 0.41 |
| 1:GE:448:TYR:HD1 | 1:GE:452:VAL:HG11 | 1.85 | 0.41 |
| 2:GF:623:LEU:HA | 2:GF:623:LEU:HD23 | 1.82 | 0.41 |
| 2:GF:903:GLY:HA3 | 3:GH:334:PHE:OXT | 2.21 | 0.41 |
| 2:GF:981:GLN:CG | 2:GF:982:LEU:N | 2.82 | 0.41 |
| 3:GG:253:LEU:HA | 3:GG:253:LEU:HD23 | 1.90 | 0.41 |
| 3:GG:310:ILE:HG13 | 3:GG:311:TYR:N | 2.36 | 0.41 |
| 3:GH:21:MET:HG3 | 3:GH:247:ILE:HG13 | 2.03 | 0.41 |
| 4:GJ:65:GLY:HA3 | 4:GJ:84:ARG:NH1 | 2.36 | 0.41 |
| 5:HB:104:VAL:HG22 | 5:HB:105:ASN:H | 1.86 | 0.41 |
| 5:HB:196:ARG:HH11 | 7:HH:5:THR:CG2 | 2.32 | 0.41 |
| 5:HB:326:MET:HB2 | 5:HB:326:MET:HE3 | 1.78 | 0.41 |
| 5:HB:365:ILE:HD13 | 5:HB:365:ILE:HG21 | 1.90 | 0.41 |
| 5:HC:144:GLU:OE1 | 5:HC:144:GLU:N | 2.54 | 0.41 |
| 5:HC:262:GLN:HA | 5:HC:381:ILE:O | 2.21 | 0.41 |
| 2:GF:220:LYS:HA | 5:HC:562:SER:OG | 2.20 | 0.41 |
| 5:HD:118:LYS:HA | 5:HD:142:ARG:CZ | 2.51 | 0.41 |
| 5:HD:120:SER:OG | 5:HD:122:VAL:HG22 | 2.21 | 0.41 |
| 5:HD:133:LEU:HA | 5:HD:133:LEU:HD23 | 1.81 | 0.41 |
| 5:HD:304:ILE:O | 5:HD:304:ILE:HD12 | 2.20 | 0.41 |
| 5:HD:89:TYR:CE1 | 5:HD:137:TYR:CZ | 3.09 | 0.41 |
| 5:HD:89:TYR:HA | 5:HD:137:TYR:CD2 | 2.55 | 0.41 |
| 6:HE:164:GLN:HE22 | 6:HG:54:SER:HA | 1.85 | 0.41 |
| 6:HF:13:ARG:HG2 | 6:HF:14:LEU:N | 2.27 | 0.41 |
| 6:HG:217:ARG:HE | 6:HG:219:ALA:C | 2.23 | 0.41 |
| 7:HH:125:LEU:O | 7:HH:129:PHE:N | 2.45 | 0.41 |
| 7:HH:232:THR:HG23 | 7:HH:235:GLU:H | 1.85 | 0.41 |
| 7:HH:470:GLY:O | 7:HJ:476:ASP:N | 2.52 | 0.41 |
| 7:HI:283:TRP:CZ3 | 7:HI:284:ASN:HB3 | 2.55 | 0.41 |
| 7:HI:343:VAL:O | 7:HI:378:ARG:NH1 | 2.49 | 0.41 |
| 7:HI:85:LEU:C | 7:HI:88:PRO:HD3 | 2.40 | 0.41 |
| 7:HJ:134:SER:N | 7:HJ:142:ILE:HD11 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HJ:233:GLN:OE1 | 7:HJ:252:GLY:HA3 | 2.21 | 0.41 |
| 7:HJ:32:VAL:O | 7:HJ:36:ILE:HG12 | 2.20 | 0.41 |
| 7:HJ:375:TYR:OH | 7:HJ:392:LEU:HD23 | 2.21 | 0.41 |
| 7:HH:399:PHE:CE2 | 7:HJ:514:PRO:HG2 | 2.55 | 0.41 |
| 5:I:359:GLU:HB3 | 5:I:370:HIS:CB | 2.37 | 0.41 |
| 5:I:81:LEU:HD22 | 5:I:143:TRP:CZ3 | 2.56 | 0.41 |
| 8:IA:91:ILE:HG22 | 8:IA:107:TYR:HB3 | 2.02 | 0.41 |
| 10:ID:213:PRO:HG3 | 10:ID:219:LEU:HD12 | 2.03 | 0.41 |
| 12:IF:112:ASP:O | 12:IF:116:MET:N | 2.41 | 0.41 |
| 12:IF:185:VAL:HG23 | 12:IF:186:THR:N | 2.35 | 0.41 |
| 5:J:144:GLU:OE1 | 5:J:144:GLU:N | 2.54 | 0.41 |
| 5:J:229:ASN:OD1 | 5:J:230:ILE:N | 2.54 | 0.41 |
| 5:J:371:PHE:HZ | 5:J:373:SER:HB3 | 1.85 | 0.41 |
| 5:K:363:ASN:HD21 | 7:BA:472:ARG:HE | 1.69 | 0.41 |
| 6:L:109:VAL:HG13 | 6:L:178:ILE:HG21 | 2.02 | 0.41 |
| 6:L:201:VAL:N | 6:L:210:THR:O | 2.31 | 0.41 |
| 6:L:74:LYS:HG3 | 6:N:70:ILE:HD11 | 2.02 | 0.41 |
| 6:N:79:PRO:HD2 | 6:N:193:TRP:CB | 2.51 | 0.41 |
| 7:O:146:SER:N | 7:O:149:GLN:HB2 | 2.35 | 0.41 |
| 7:O:451:PHE:CE1 | 7:O:470:GLY:HA2 | 2.55 | 0.41 |
| 7:P:231:GLY:O | 7:P:249:THR:HG21 | 2.21 | 0.41 |
| 7:P:283:TRP:CZ3 | 7:P:284:ASN:HB3 | 2.55 | 0.41 |
| 7:P:453:GLU:HG3 | 7:P:475:LEU:HD11 | 2.03 | 0.41 |
| 7:P:491:ASP:HB2 | 7:P:496:ARG:HG2 | 2.01 | 0.41 |
| 7:Q:375:TYR:OH | 7:Q:392:LEU:HD23 | 2.21 | 0.41 |
| 7:P:476:ASP:OD2 | 7:Q:454:HIS:HE1 | 2.04 | 0.41 |
| 8:R:14:ASP:CG | 8:R:17:ARG:HH22 | 2.18 | 0.41 |
| 8:S:49:ILE:HG23 | 8:S:60:VAL:O | 2.21 | 0.41 |
| 1:X:123:ILE:HA | 1:X:123:ILE:HD12 | 1.76 | 0.41 |
| 1:X:507:ASP:HA | 1:X:597:TYR:CZ | 2.56 | 0.41 |
| 1:X:448:TYR:CE2 | 1:X:642:PHE:HB2 | 2.55 | 0.41 |
| 1:Y:145:PHE:CD1 | 1:Y:169:GLN:HA | 2.56 | 0.41 |
| 1:Y:46:TYR:HB3 | 1:Y:53:LEU:HD23 | 2.02 | 0.41 |
| 13:YA:227[A]:ARG:HG2 | 13:YA:228[A]:GLU:N | 2.36 | 0.41 |
| 13:YA:399[F]:HIS:ND1 | 13:YA:417[F]:PRO:HD3 | 2.36 | 0.41 |
| 13:YA:399[B]:HIS:ND1 | 13:YA:417[B]:PRO:HD3 | 2.36 | 0.41 |
| 13:YA:552[E]:GLU:HB2 | 13:YB:544[E]:TRP:HB2 | 2.03 | 0.41 |
| 13:YB:239[C]:GLU:H | 13:YB:239[C]:GLU:CD | 2.24 | 0.41 |
| 13:YB:266[C]:TRP:NE1 | 13:YB:274[C]:GLN:HG2 | 2.36 | 0.41 |
| 13:YB:336[B]:LEU:HA | 13:YB:336[B]:LEU:HD12 | 1.85 | 0.41 |
| 13:YB:399[E]:HIS:ND1 | 13:YB:417[E]:PRO:HD3 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:393[E]:MET:O | 13:YB:400[E]:ILE:HA | 2.21 | 0.41 |
| 13:YB:506[D]:VAL:HG21 | 13:YC:502[D]:VAL:HG21 | 2.03 | 0.41 |
| 13:YB:554[C]:MET:HE3 | 13:YB:554[C]:MET:HB3 | 1.92 | 0.41 |
| 13:YB:558[D]:SER:O | 13:YC:551[D]:THR:HA | 2.21 | 0.41 |
| 13:YB:558[E]:SER:O | 13:YC:551[E]:THR:HA | 2.21 | 0.41 |
| 13:YB:73[E]:VAL:HG21 | 13:YC:129[E]:THR:HG22 | 2.03 | 0.41 |
| 13:YC:454[F]:LYS:C | 13:YC:455[F]:LYS:HG3 | 2.40 | 0.41 |
| 13:YB:515[C]:LYS:HG3 | 13:YC:507[C]:GLU:HA | 2.02 | 0.41 |
| 13:YB:552[E]:GLU:CB | 13:YC:544[E]:TRP:HB2 | 2.51 | 0.41 |
| 13:YB:558[F]:SER:O | 13:YC:551[F]:THR:HA | 2.21 | 0.41 |
| 13:YA:553[D]:LYS:HA | 13:YC:560[D]:ILE:O | 2.21 | 0.41 |
| 13:YC:76[B]:PRO:HB2 | 13:YC:98[B]:GLY:O | 2.21 | 0.41 |
| 13:YC:81[E]:ARG:HD3 | 14:YE:261[E]:SER:HA | 2.03 | 0.41 |
| 14:YD:26[F]:ASN:ND2 | 14:YD:26[F]:ASN:O | 2.53 | 0.41 |
| 14:YE:51[C]:MET:SD | 14:YE:108[C]:GLU:HA | 2.61 | 0.41 |
| 14:YE:290[B]:ASN:OD1 | 14:YE:290[B]:ASN:C | 2.58 | 0.41 |
| 14:YE:209[F]:TYR:HB3 | 14:YE:324[F]:ILE:HG12 | 2.03 | 0.41 |
| 14:YE:345[B]:GLU:HB3 | 14:YE:352[B]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:10[B]:PRO:HB2 | 14:YE:74[B]:VAL:HG21 | 2.03 | 0.41 |
| 14:YF:51[E]:MET:SD | 14:YF:108[E]:GLU:HA | 2.61 | 0.41 |
| 14:YF:15[A]:LYS:HB3 | 14:YF:15[A]:LYS:HE2 | 1.54 | 0.41 |
| 14:YF:259[E]:LEU:HA | 14:YF:259[E]:LEU:HD23 | 1.83 | 0.41 |
| 14:YF:345[A]:GLU:HB3 | 14:YF:352[A]:VAL:HG13 | 2.03 | 0.41 |
| 14:YF:345[B]:GLU:HB3 | 14:YF:352[B]:VAL:HG13 | 2.03 | 0.41 |
| 14:YF:10[A]:PRO:HB2 | 14:YF:74[A]:VAL:HG21 | 2.03 | 0.41 |
| 14:YF:86[F]:ARG:HD2 | 14:YF:192[F]:ILE:HD12 | 2.02 | 0.41 |
| 2:Z:151:PHE:HB3 | 2:Z:166:PHE:CZ | 2.55 | 0.41 |
| 2:Z:224:LEU:O | 2:Z:224:LEU:HD23 | 2.21 | 0.41 |
| 2:Z:376:PHE:HB2 | 2:Z:405:VAL:HA | 2.02 | 0.41 |
| 2:Z:593:GLU:HB3 | 2:Z:594:ILE:H | 1.61 | 0.41 |
| 2:Z:600:PHE:CE2 | 2:Z:604:VAL:HB | 2.56 | 0.41 |
| 2:Z:78:TYR:O | 2:Z:99:GLU:HB2 | 2.21 | 0.41 |
| 1:A:337:GLN:O | 1:A:348:PHE:HZ | 2.02 | 0.41 |
| 1:A:418:THR:HG22 | 1:A:482:ILE:HG22 | 2.02 | 0.41 |
| 1:A:99:LEU:HD12 | 1:A:99:LEU:O | 2.21 | 0.41 |
| 5:AD:137:TYR:HB2 | 5:AD:143:TRP:HE1 | 1.85 | 0.41 |
| 5:AD:338:ASP:HB3 | 5:AD:349:TRP:CD1 | 2.56 | 0.41 |
| 5:AC:542:LEU:HD21 | 5:AD:569:TYR:CZ | 2.55 | 0.41 |
| 5:AD:54:ALA:HB2 | 5:AD:71:ASN:O | 2.20 | 0.41 |
| 5:AE:313:PHE:HE2 | 5:AE:320:LEU:HD21 | 1.84 | 0.41 |
| 5:AE:323:THR:CG2 | 5:AE:359:GLU:HB2 | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:304:ILE:HG23 | 5:AE:385:TRP:CD1 | 2.56 | 0.41 |
| 5:AE:399:ILE:O | 5:AE:402:GLU:HB3 | 2.20 | 0.41 |
| 5:AE:84:GLY:C | 5:AE:86:VAL:H | 2.17 | 0.41 |
| 6:AF:12:SER:HA | 6:AH:6:ASN:O | 2.21 | 0.41 |
| 6:AF:200:THR:HA | 6:AF:211:VAL:HA | 2.03 | 0.41 |
| 6:AH:200:THR:HA | 6:AH:211:VAL:HA | 2.03 | 0.41 |
| 7:AJ:343:VAL:HG13 | 7:AJ:524:LYS:O | 2.20 | 0.41 |
| 1:B:46:TYR:HB3 | 1:B:53:LEU:HD23 | 2.02 | 0.41 |
| 7:BA:166:GLN:O | 7:BA:170:ILE:HB | 2.20 | 0.41 |
| 7:BA:375:TYR:OH | 7:BA:392:LEU:HD23 | 2.21 | 0.41 |
| 7:AJ:516:ASN:OD1 | 7:BA:438:GLN:HB2 | 2.20 | 0.41 |
| 7:AJ:515:TRP:CZ3 | 7:BA:439:ILE:HG12 | 2.56 | 0.41 |
| 9:BD:58:SER:HB3 | 9:BD:61:LEU:HB3 | 2.03 | 0.41 |
| 1:BH:243:ILE:HD13 | 1:BH:243:ILE:HG21 | 1.90 | 0.41 |
| 1:BH:328:LEU:HA | 1:BH:328:LEU:HD23 | 1.71 | 0.41 |
| 1:BH:52:ARG:HG2 | 1:BI:42:GLU:OE1 | 2.21 | 0.41 |
| 1:BH:69:GLN:HE21 | 11:DI:25:MET:HE1 | 1.86 | 0.41 |
| 1:BI:322:ILE:HG13 | 1:BI:323:GLU:N | 2.35 | 0.41 |
| 1:BI:414:LEU:O | 1:BI:415:PHE:HD1 | 2.04 | 0.41 |
| 1:BI:494:THR:HG22 | 1:BI:498:GLY:HA2 | 2.03 | 0.41 |
| 1:BI:608:LYS:HD3 | 2:BJ:802:TYR:CE1 | 2.56 | 0.41 |
| 2:BJ:186:ASP:HB3 | 2:BJ:189:ARG:HG3 | 2.03 | 0.41 |
| 2:BJ:206:GLN:HA | 2:BJ:207:PRO:HD2 | 2.00 | 0.41 |
| 2:BJ:217:GLN:HG2 | 2:BJ:218:THR:N | 2.36 | 0.41 |
| 2:BJ:31:ASN:O | 2:BJ:32:PHE:HD1 | 2.04 | 0.41 |
| 2:BJ:379:ILE:HD11 | 2:BJ:402:GLY:H | 1.86 | 0.41 |
| 2:BJ:442:SER:HA | 2:BJ:491:ILE:HD13 | 2.03 | 0.41 |
| 2:BJ:528:ASN:ND2 | 3:ED:285:PRO:HB2 | 2.35 | 0.41 |
| 2:C:425:ARG:NH2 | 2:C:449:LYS:HG2 | 2.36 | 0.41 |
| 2:C:447:ASN:OD1 | 2:C:448:PHE:N | 2.54 | 0.41 |
| 2:C:472:LYS:HG3 | 2:C:474:GLU:HG3 | 2.03 | 0.41 |
| 2:C:683:TYR:O | 2:C:686:LEU:N | 2.53 | 0.41 |
| 2:C:899:PHE:O | 2:C:900:ILE:HD13 | 2.21 | 0.41 |
| 3:CA:96:GLY:HA2 | 3:CA:103:PRO:CB | 2.50 | 0.41 |
| 3:CA:60:TYR:HA | 3:CA:61:PRO:HD3 | 1.94 | 0.41 |
| 3:CA:38:PHE:HE1 | 3:CA:80:LYS:HG3 | 1.86 | 0.41 |
| 3:CB:238:LEU:HA | 3:CB:238:LEU:HD12 | 1.88 | 0.41 |
| 4:CC:166:SER:OG | 4:CE:173:SER:N | 2.39 | 0.41 |
| 4:CD:60:ILE:HB | 4:CE:4:GLN:NE2 | 2.36 | 0.41 |
| 5:CF:304:ILE:HD12 | 5:CF:384:THR:O | 2.21 | 0.41 |
| 5:CG:552:VAL:HG22 | 5:CG:553:GLY:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:CH:104:VAL:HG22 | 5:CH:105:ASN:N | 2.35 | 0.41 |
| 5:CH:150:GLN:HG3 | 5:CH:152:ASP:HB3 | 2.01 | 0.41 |
| 5:CH:290:SER:HB3 | 5:CH:370:HIS:HA | 2.01 | 0.41 |
| 6:CJ:200:THR:HA | 6:CJ:211:VAL:HA | 2.03 | 0.41 |
| 7:DB:127:ASN:O | 7:DB:131:THR:HG23 | 2.20 | 0.41 |
| 7:DB:143:LYS:HG2 | 7:DC:138:SER:C | 2.41 | 0.41 |
| 7:DB:19:ASP:HB3 | 7:DD:33:GLN:OE1 | 2.21 | 0.41 |
| 7:DC:63:GLU:O | 7:DC:66:VAL:HG22 | 2.21 | 0.41 |
| 7:DD:453:GLU:HG3 | 7:DD:475:LEU:HD21 | 2.02 | 0.41 |
| 7:DB:465:ARG:HG2 | 7:DD:480:ARG:HG3 | 2.03 | 0.41 |
| 7:DB:510:ASN:O | 7:DD:504:ARG:NH1 | 2.54 | 0.41 |
| 7:DB:399:PHE:CE2 | 7:DD:514:PRO:HG2 | 2.55 | 0.41 |
| 7:DB:52:SER:N | 7:DD:60:ILE:HG22 | 2.35 | 0.41 |
| 8:DE:91:ILE:HG22 | 8:DE:107:TYR:HB3 | 2.02 | 0.41 |
| 8:DE:10:PHE:O | 8:DE:12:SER:N | 2.54 | 0.41 |
| 11:DI:174:LYS:O | 11:DI:177:ILE:HG22 | 2.21 | 0.41 |
| 11:DI:36:PHE:CD1 | 11:DI:180:PHE:HZ | 2.39 | 0.41 |
| 1:EA:201:VAL:HG21 | 1:EA:262:PRO:HB3 | 2.02 | 0.41 |
| 1:EA:360:VAL:HG23 | 1:EA:375:ALA:O | 2.20 | 0.41 |
| 1:EA:433:GLU:OE2 | 1:EA:655:LEU:HD11 | 2.20 | 0.41 |
| 1:EA:59:LEU:CD1 | 1:EB:37:LEU:HD12 | 2.50 | 0.41 |
| 1:EA:657:PRO:O | 1:EA:658:ILE:HD13 | 2.21 | 0.41 |
| 1:EB:596:ASN:N | 1:EB:596:ASN:OD1 | 2.53 | 0.41 |
| 2:EC:1012:LEU:HD12 | 2:EC:1012:LEU:O | 2.21 | 0.41 |
| 2:EC:28:VAL:HG23 | 2:EC:29:GLY:N | 2.35 | 0.41 |
| 2:EC:417:PHE:CE1 | 2:EC:423:GLU:HG2 | 2.56 | 0.41 |
| 2:EC:447:ASN:OD1 | 2:EC:448:PHE:N | 2.54 | 0.41 |
| 2:EC:516:TRP:HE1 | 2:EC:518:LYS:HG2 | 1.85 | 0.41 |
| 2:EC:644:ASP:HB2 | 2:EC:646:ARG:HG2 | 2.02 | 0.41 |
| 2:EC:861:TYR:HE2 | 2:EC:863:VAL:HG22 | 1.86 | 0.41 |
| 4:EF:222:LEU:HD13 | 4:EH:216:THR:CG2 | 2.51 | 0.41 |
| 5:EI:67:SER:HA | 5:EI:94:ARG:O | 2.20 | 0.41 |
| 5:EJ:303:PRO:HD2 | 5:EJ:365:ILE:HD13 | 2.02 | 0.41 |
| 5:FA:264:ARG:HH12 | 6:FB:2:SER:N | 2.19 | 0.41 |
| 6:FB:42:GLN:N | 6:FB:42:GLN:OE1 | 2.52 | 0.41 |
| 6:FC:79:PRO:HD2 | 6:FC:193:TRP:CB | 2.51 | 0.41 |
| 6:FD:195:LEU:HA | 6:FD:215:PHE:HD1 | 1.85 | 0.41 |
| 6:FD:88:TRP:HB3 | 6:FD:90:PHE:CE1 | 2.55 | 0.41 |
| 7:FE:259:MET:HG2 | 7:FE:260:ARG:O | 2.21 | 0.41 |
| 7:FF:196:VAL:HA | 7:FF:199:VAL:HG22 | 2.03 | 0.41 |
| 7:FF:231:GLY:O | 7:FF:249:THR:HG21 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FG:351:ALA:O | 7:FG:520:ASN:ND2 | 2.54 | 0.41 |
| 8:FH:10:PHE:O | 8:FH:12:SER:N | 2.54 | 0.41 |
| 4:G:131:LYS:HD3 | 4:G:161:ASN:HD22 | 1.85 | 0.41 |
| 12:GC:113:PHE:CE1 | 12:GC:170:ASN:HA | 2.56 | 0.41 |
| 1:GD:227:ARG:NH2 | 1:GE:81:ARG:HH21 | 2.19 | 0.41 |
| 1:GD:472:ASP:O | 1:GD:474:SER:N | 2.54 | 0.41 |
| 1:GD:414:LEU:HD21 | 1:GD:486:ARG:HH21 | 1.85 | 0.41 |
| 1:GD:580:LEU:HD12 | 1:GD:580:LEU:C | 2.41 | 0.41 |
| 2:GF:186:ASP:HB3 | 2:GF:189:ARG:HG3 | 2.03 | 0.41 |
| 2:GF:600:PHE:CE2 | 2:GF:604:VAL:HB | 2.56 | 0.41 |
| 2:GF:861:TYR:HE2 | 2:GF:863:VAL:HG22 | 1.86 | 0.41 |
| 3:GG:114:CYS:HA | 3:GG:120:ASN:HD21 | 1.85 | 0.41 |
| 3:GG:284:HIS:HA | 3:GG:285:PRO:HD3 | 1.94 | 0.41 |
| 4:GJ:131:LYS:HD3 | 4:GJ:161:ASN:HD22 | 1.85 | 0.41 |
| 5:HB:139:ALA:HB3 | 5:HC:99:PHE:CB | 2.51 | 0.41 |
| 5:HB:151:ILE:O | 5:HB:152:ASP:HB3 | 2.21 | 0.41 |
| 5:HB:304:ILE:HG12 | 5:HB:305:ASN:O | 2.20 | 0.41 |
| 5:HC:104:VAL:HG13 | 5:HC:105:ASN:H | 1.85 | 0.41 |
| 5:HC:357:SER:HB3 | 5:HC:358:VAL:H | 1.64 | 0.41 |
| 5:HC:397:ASP:OD1 | 5:HC:398:GLU:HG2 | 2.21 | 0.41 |
| 5:HD:261:ARG:HA | 5:HD:261:ARG:HD3 | 1.91 | 0.41 |
| 5:HC:482:GLY:O | 5:HD:489:GLY:HA3 | 2.21 | 0.41 |
| 5:HC:340:VAL:HG22 | 6:HG:173:THR:HA | 2.02 | 0.41 |
| 6:HG:195:LEU:HA | 6:HG:215:PHE:HD1 | 1.85 | 0.41 |
| 7:HH:456:ASP:CB | 7:HH:462:ASN:HD21 | 2.34 | 0.41 |
| 7:HI:17:LYS:HD2 | 7:HI:18:PHE:H | 1.86 | 0.41 |
| 7:HI:212:PRO:CB | 7:HJ:199:VAL:HA | 2.43 | 0.41 |
| 7:HH:19:ASP:HB3 | 7:HJ:33:GLN:OE1 | 2.20 | 0.41 |
| 7:HJ:417:ASN:O | 7:HJ:424:ARG:NH1 | 2.53 | 0.41 |
| 7:HH:443:SER:HA | 7:HJ:509:GLY:O | 2.21 | 0.41 |
| 7:HJ:351:ALA:O | 7:HJ:520:ASN:ND2 | 2.54 | 0.41 |
| 7:HJ:99:ARG:O | 7:HJ:114:SER:HA | 2.21 | 0.41 |
| 8:IB:69:TRP:HB2 | 8:IB:159:LEU:HD23 | 2.03 | 0.41 |
| 9:IC:58:SER:HB3 | 9:IC:61:LEU:HB3 | 2.03 | 0.41 |
| 11:IE:36:PHE:CD1 | 11:IE:180:PHE:HZ | 2.39 | 0.41 |
| 5:J:11:VAL:HG22 | 5:K:20:ARG:NE | 2.36 | 0.41 |
| 7:O:171:LYS:HA | 7:O:174:ALA:HB3 | 2.03 | 0.41 |
| 7:O:375:TYR:CE2 | 7:O:390:PRO:HB2 | 2.53 | 0.41 |
| 7:P:491:ASP:HB2 | 7:P:496:ARG:CG | 2.51 | 0.41 |
| 7:O:503:ASN:HD21 | 7:Q:446:LYS:H | 1.69 | 0.41 |
| 7:P:75:ALA:HB1 | 7:Q:75:ALA:HB1 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Q:77:THR:OG1 | 7:Q:78:PRO:HD2 | 2.20 | 0.41 |
| 12:W:113:PHE:CE1 | 12:W:170:ASN:HA | 2.56 | 0.41 |
| 1:X:178:ILE:HD11 | 1:X:265:ASN:O | 2.21 | 0.41 |
| 1:X:105:ALA:HB2 | 1:X:275:THR:HG21 | 2.02 | 0.41 |
| 1:X:429:LEU:O | 1:X:429:LEU:HD12 | 2.21 | 0.41 |
| 1:X:99:LEU:O | 1:X:99:LEU:HD12 | 2.21 | 0.41 |
| 1:Y:347:THR:OG1 | 1:Y:348:PHE:N | 2.54 | 0.41 |
| 1:Y:88:SER:O | 1:Y:91:GLN:HB3 | 2.21 | 0.41 |
| 13:YA:227[B]:ARG:HG2 | 13:YA:228[B]:GLU:N | 2.36 | 0.41 |
| 13:YA:336[B]:LEU:HD12 | 13:YA:336[B]:LEU:HA | 1.85 | 0.41 |
| 13:YA:60[B]:PRO:HB3 | 13:YB:60[B]:PRO:HB3 | 2.02 | 0.41 |
| 13:YA:83[E]:TYR:OH | 13:YA:85[E]:HIS:HE1 | 2.04 | 0.41 |
| 13:YB:227[E]:ARG:HG2 | 13:YB:228[E]:GLU:N | 2.36 | 0.41 |
| 13:YB:296[D]:LEU:HA | 13:YB:296[D]:LEU:HD12 | 1.85 | 0.41 |
| 13:YB:34[F]:LEU:HD13 | 14:YE:163[F]:THR:CG2 | 2.47 | 0.41 |
| 13:YB:450[F]:VAL:HG11 | 13:YC:446[F]:GLY:N | 2.36 | 0.41 |
| 13:YB:453[B]:ASP:O | 13:YC:445[B]:ASP:HA | 2.20 | 0.41 |
| 13:YB:453[E]:ASP:O | 13:YC:445[E]:ASP:HA | 2.20 | 0.41 |
| 13:YB:490[F]:VAL:HG21 | 13:YC:486[F]:GLU:HB2 | 2.03 | 0.41 |
| 13:YA:552[A]:GLU:HB2 | 13:YB:544[A]:TRP:HB2 | 2.03 | 0.41 |
| 13:YB:76[B]:PRO:HB2 | 13:YB:98[B]:GLY:O | 2.21 | 0.41 |
| 13:YC:239[A]:GLU:CD | 13:YC:239[A]:GLU:H | 2.24 | 0.41 |
| 13:YB:454[B]:LYS:NZ | 13:YC:464[B]:TYR:OH | 2.53 | 0.41 |
| 13:YB:515[A]:LYS:HG3 | 13:YC:507[A]:GLU:HA | 2.02 | 0.41 |
| 13:YC:66[C]:MET:HA | 13:YC:66[C]:MET:HE3 | 2.02 | 0.41 |
| 13:YC:83[E]:TYR:OH | 13:YC:85[E]:HIS:HE1 | 2.04 | 0.41 |
| 14:YD:212[F]:ILE:HG12 | 14:YD:228[F]:TYR:HB2 | 2.02 | 0.41 |
| 10:DH:286:VAL:HG13 | 14:YE:100[D]:LYS:HE2 | 2.03 | 0.41 |
| 14:YE:136[F]:LEU:HD21 | 14:YE:166[F]:PHE:CE2 | 2.56 | 0.41 |
| 14:YE:145[A]:LEU:HG | 14:YE:145[A]:LEU:H | 1.70 | 0.41 |
| 14:YE:170[E]:LEU:HA | 14:YE:170[E]:LEU:HD23 | 1.69 | 0.41 |
| 13:YB:93[B]:ASN:OD1 | 14:YE:280[B]:SER:HB2 | 2.21 | 0.41 |
| 14:YE:345[A]:GLU:HB3 | 14:YE:352[A]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:345[C]:GLU:HB3 | 14:YE:352[C]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:345[E]:GLU:HB3 | 14:YE:352[E]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:345[F]:GLU:HB3 | 14:YE:352[F]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:75[B]:ALA:HB2 | 14:YE:83[B]:VAL:HA | 2.01 | 0.41 |
| 14:YE:75[C]:ALA:HB2 | 14:YE:83[C]:VAL:HA | 2.02 | 0.41 |
| 14:YF:10[B]:PRO:HB2 | 14:YF:74[B]:VAL:HG21 | 2.03 | 0.41 |
| 14:YF:136[D]:LEU:HD21 | 14:YF:166[D]:PHE:CE2 | 2.56 | 0.41 |
| 14:YF:170[C]:LEU:HA | 14:YF:170[C]:LEU:HD23 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:174[F]:ARG:HG3 | 14:YF:188[F]:VAL:HG22 | 2.03 | 0.41 |
| 14:YF:210[B]:PRO:HB2 | 14:YF:228[B]:TYR:CD2 | 2.56 | 0.41 |
| 14:YF:44[C]:LEU:HD23 | 14:YF:44[C]:LEU:HA | 1.85 | 0.41 |
| 2:Z:300:LEU:N | 2:Z:301:PRO:CD | 2.84 | 0.41 |
| 2:Z:315:ASP:O | 2:Z:316:ASP:HB2 | 2.20 | 0.41 |
| 2:Z:174:HIS:HB3 | 2:Z:535:VAL:HB | 2.03 | 0.41 |
| 2:Z:548:ILE:O | 2:Z:555:ARG:NH2 | 2.54 | 0.41 |
| 2:Z:659:LEU:HB3 | 2:Z:660:GLN:H | 1.69 | 0.41 |
| 2:Z:793:CYS:HB3 | 2:Z:813:ILE:HG21 | 2.03 | 0.41 |
| 15:ZA:26[E]:GLN:HE21 | 15:ZA:26[E]:GLN:HB2 | 1.73 | 0.41 |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:HA | 1.77 | 0.41 |
| 1:A:222:THR:O | 1:A:223:ILE:HG12 | 2.21 | 0.41 |
| 1:A:175:THR:O | 1:A:270:ILE:HG22 | 2.20 | 0.41 |
| 1:A:278:ALA:H | 1:A:316:GLY:HA2 | 1.85 | 0.41 |
| 1:A:347:THR:O | 1:A:351:GLU:N | 2.43 | 0.41 |
| 1:A:580:LEU:C | 1:A:580:LEU:HD12 | 2.41 | 0.41 |
| 4:AA:35:PHE:CD1 | 4:AA:39:TYR:HE2 | 2.39 | 0.41 |
| 4:AB:213:LYS:HE3 | 4:AB:249:ILE:HG12 | 2.03 | 0.41 |
| 5:AC:103:ASN:CG | 5:AC:104:VAL:H | 2.24 | 0.41 |
| 5:AC:160:SER:HB3 | 5:AD:161:ASN:ND2 | 2.21 | 0.41 |
| 5:AC:279:SER:HB2 | 5:AE:326:MET:HB2 | 2.03 | 0.41 |
| 5:AD:181:PHE:HE2 | 5:AD:246:THR:HG22 | 1.86 | 0.41 |
| 5:AE:120:SER:OG | 5:AE:122:VAL:HG22 | 2.21 | 0.41 |
| 5:AE:177:PHE:O | 5:AE:230:ILE:HG13 | 2.21 | 0.41 |
| 5:AE:258:TYR:HD1 | 5:AE:386:PHE:HD1 | 1.67 | 0.41 |
| 5:AD:443:PHE:O | 5:AE:408:VAL:HG13 | 2.21 | 0.41 |
| 6:AF:195:LEU:HA | 6:AF:215:PHE:HD1 | 1.85 | 0.41 |
| 7:AI:125:LEU:HD11 | 7:AJ:125:LEU:HG | 2.03 | 0.41 |
| 7:AI:456:ASP:CB | 7:AI:462:ASN:HD21 | 2.34 | 0.41 |
| 7:AJ:283:TRP:CZ3 | 7:AJ:284:ASN:HB3 | 2.55 | 0.41 |
| 7:AJ:358:ALA:HB1 | 7:AJ:524:LYS:HE3 | 2.02 | 0.41 |
| 7:AJ:479:ASN:HB2 | 7:BA:469:VAL:O | 2.21 | 0.41 |
| 1:B:229:THR:OG1 | 1:B:233:ASN:OD1 | 2.34 | 0.41 |
| 7:AJ:335:ASN:N | 7:BA:329:ASN:HD21 | 2.19 | 0.41 |
| 7:BA:417:ASN:O | 7:BA:424:ARG:NH1 | 2.53 | 0.41 |
| 11:BF:174:LYS:O | 11:BF:177:ILE:HG22 | 2.21 | 0.41 |
| 1:BH:465:LEU:HA | 1:BH:465:LEU:HD23 | 1.89 | 0.41 |
| 2:BJ:1014:ASP:OD1 | 2:BJ:1015:ASN:N | 2.53 | 0.41 |
| 2:BJ:573:VAL:CG2 | 2:BJ:610:ILE:HB | 2.51 | 0.41 |
| 2:BJ:947:VAL:HA | 3:CA:118:PRO:CB | 2.44 | 0.41 |
| 2:C:206:GLN:C | 2:C:208:VAL:N | 2.75 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:217:GLN:HG2 | 2:C:218:THR:H | 1.85 | 0.41 |
| 2:C:306:ARG:C | 2:C:307:ILE:HD12 | 2.41 | 0.41 |
| 2:C:307:ILE:HG22 | 2:C:308:ALA:N | 2.36 | 0.41 |
| 2:C:196:GLU:HB3 | 2:C:520:SER:OG | 2.21 | 0.41 |
| 2:C:584:GLY:HA2 | 2:C:600:PHE:CB | 2.46 | 0.41 |
| 2:C:921:TRP:N | 2:C:921:TRP:CD1 | 2.85 | 0.41 |
| 3:CA:197:ASP:OD1 | 3:CA:197:ASP:N | 2.54 | 0.41 |
| 3:CB:147:LEU:CD2 | 3:CB:152:GLU:HG3 | 2.51 | 0.41 |
| 3:CB:331:LEU:HA | 3:CB:331:LEU:HD23 | 1.73 | 0.41 |
| 4:CC:65:GLY:HA3 | 4:CC:84:ARG:NH1 | 2.36 | 0.41 |
| 4:CE:131:LYS:HD3 | 4:CE:161:ASN:HD22 | 1.85 | 0.41 |
| 5:CF:153:LYS:HG2 | 5:CF:154:ILE:N | 2.36 | 0.41 |
| 5:CF:271:THR:HB | 5:CF:273:LYS:HG2 | 2.03 | 0.41 |
| 5:CG:397:ASP:OD1 | 5:CG:398:GLU:HG2 | 2.21 | 0.41 |
| 5:CH:409:SER:OG | 5:CH:411:GLY:N | 2.52 | 0.41 |
| 6:CI:82:VAL:HG23 | 6:CI:187:LYS:HE3 | 2.02 | 0.41 |
| 6:CI:70:ILE:HD12 | 6:CI:196:LEU:HD11 | 2.03 | 0.41 |
| 3:D:255:SER:O | 3:D:258:PHE:N | 2.53 | 0.41 |
| 7:DB:216:MET:HG3 | 7:DB:217:ASN:N | 2.36 | 0.41 |
| 7:DB:255:SER:N | 7:DB:278:SER:OG | 2.53 | 0.41 |
| 7:DB:456:ASP:CB | 7:DB:462:ASN:HD21 | 2.34 | 0.41 |
| 7:DC:240:ASN:HB3 | 7:DC:243:VAL:HG22 | 2.03 | 0.41 |
| 7:DB:439:ILE:HG12 | 7:DD:515:TRP:CZ3 | 2.56 | 0.41 |
| 7:DC:77:THR:HG21 | 7:DD:72:ASN:CG | 2.41 | 0.41 |
| 8:DF:10:PHE:O | 8:DF:12:SER:N | 2.54 | 0.41 |
| 8:DE:118:ARG:NH2 | 8:DF:62:GLY:O | 2.54 | 0.41 |
| 9:DG:62:PHE:HZ | 9:DG:127:ALA:HA | 1.86 | 0.41 |
| 9:DG:20:ASN:HA | 1:EB:311:VAL:CG1 | 2.42 | 0.41 |
| 10:DH:35:THR:HA | 10:DH:126:ASN:O | 2.21 | 0.41 |
| 11:DI:166:LEU:HD23 | 11:DI:166:LEU:HA | 1.83 | 0.41 |
| 11:DI:9:ILE:HG12 | 11:DI:10:GLU:O | 2.21 | 0.41 |
| 12:BG:215:MET:CE | 12:DJ:99:SER:HB2 | 2.50 | 0.41 |
| 1:EA:178:ILE:HD11 | 1:EA:265:ASN:O | 2.21 | 0.41 |
| 1:EA:414:LEU:HD21 | 1:EA:486:ARG:HH21 | 1.85 | 0.41 |
| 1:EB:158:ASN:ND2 | 1:EB:160:GLN:HG2 | 2.35 | 0.41 |
| 1:EB:378:PRO:HG2 | 1:EB:381:GLY:O | 2.21 | 0.41 |
| 1:EB:394:ASN:O | 1:EB:397:LYS:HG2 | 2.21 | 0.41 |
| 1:EB:92:ALA:O | 1:EB:95:ASP:N | 2.54 | 0.41 |
| 2:EC:145:ALA:HB2 | 2:EC:542:THR:CB | 2.48 | 0.41 |
| 2:EC:319:TYR:CD2 | 2:EC:375:VAL:HG21 | 2.56 | 0.41 |
| 2:EC:31:ASN:O | 2:EC:32:PHE:HD1 | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:EC:472:LYS:HG3 | 2:EC:474:GLU:HG3 | 2.03 | 0.41 |
| 2:EC:852:ILE:HG21 | 2:EC:854:TYR:CZ | 2.56 | 0.41 |
| 2:EC:33:TYR:CE1 | 2:EC:85:ALA:HB3 | 2.55 | 0.41 |
| 4:EF:25:PHE:HB2 | 4:EG:15:ILE:HD13 | 2.03 | 0.41 |
| 4:EF:65:GLY:HA3 | 4:EF:84:ARG:NH1 | 2.36 | 0.41 |
| 5:EI:128:VAL:HB | 5:EI:131:SER:OG | 2.21 | 0.41 |
| 5:EJ:104:VAL:HG13 | 5:EJ:105:ASN:H | 1.85 | 0.41 |
| 5:EJ:323:THR:HG21 | 5:EJ:354:THR:HG23 | 2.02 | 0.41 |
| 5:EJ:371:PHE:HZ | 5:EJ:373:SER:HB3 | 1.85 | 0.41 |
| 5:FA:102:TRP:N | 5:FA:102:TRP:CD1 | 2.83 | 0.41 |
| 5:FA:104:VAL:HG22 | 5:FA:105:ASN:N | 2.35 | 0.41 |
| 5:FA:304:ILE:HG23 | 5:FA:385:TRP:CD1 | 2.56 | 0.41 |
| 6:FB:200:THR:HA | 6:FB:211:VAL:HA | 2.03 | 0.41 |
| 6:FB:82:VAL:HG23 | 6:FB:187:LYS:HE3 | 2.02 | 0.41 |
| 6:FD:79:PRO:HD2 | 6:FD:193:TRP:CB | 2.51 | 0.41 |
| 7:FE:49:ASP:OD1 | 7:FE:50:ALA:N | 2.54 | 0.41 |
| 7:FE:52:SER:N | 7:FG:60:ILE:HG22 | 2.35 | 0.41 |
| 7:FF:350:ALA:HB1 | 7:FG:383:TYR:OH | 2.21 | 0.41 |
| 7:FE:475:LEU:HA | 7:FF:470:GLY:O | 2.20 | 0.41 |
| 7:FF:479:ASN:HB2 | 7:FG:469:VAL:O | 2.20 | 0.41 |
| 7:FF:212:PRO:CB | 7:FG:199:VAL:HA | 2.42 | 0.41 |
| 4:F:173:SER:N | 4:G:166:SER:OG | 2.41 | 0.41 |
| 11:GB:50:ILE:HD11 | 11:GB:169:ILE:CD1 | 2.51 | 0.41 |
| 12:GC:171:TYR:HD1 | 12:GC:239:PHE:CE2 | 2.38 | 0.41 |
| 1:GD:222:THR:O | 1:GD:223:ILE:HG12 | 2.21 | 0.41 |
| 1:GD:448:TYR:CE2 | 1:GD:642:PHE:HB2 | 2.55 | 0.41 |
| 1:GD:657:PRO:O | 1:GD:658:ILE:HD13 | 2.21 | 0.41 |
| 1:GE:448:TYR:HA | 1:GE:452:VAL:CG1 | 2.49 | 0.41 |
| 1:GE:464:MET:HG3 | 1:GE:465:LEU:N | 2.36 | 0.41 |
| 1:GE:596:ASN:OD1 | 1:GE:596:ASN:N | 2.53 | 0.41 |
| 1:GE:66:TYR:O | 1:GE:69:GLN:N | 2.54 | 0.41 |
| 2:GF:307:ILE:HG22 | 2:GF:308:ALA:N | 2.36 | 0.41 |
| 2:GF:484:HIS:O | 2:GF:485:TYR:HB3 | 2.21 | 0.41 |
| 2:GF:526:ILE:HA | 2:GF:526:ILE:HD12 | 1.84 | 0.41 |
| 2:GF:683:TYR:O | 2:GF:686:LEU:N | 2.53 | 0.41 |
| 2:GF:947:VAL:HB | 3:GG:119:TYR:HD2 | 1.86 | 0.41 |
| 2:GF:958:MET:O | 2:GF:961:VAL:HG23 | 2.21 | 0.41 |
| 2:GF:78:TYR:O | 2:GF:99:GLU:HB2 | 2.21 | 0.41 |
| 3:GG:71:MET:HG2 | 3:GG:309:MET:CE | 2.51 | 0.41 |
| 3:GG:64:SER:OG | 3:GG:67:GLY:N | 2.36 | 0.41 |
| 3:GH:80:LYS:HG2 | 3:GH:81:VAL:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HB:133:LEU:HA | 5:HB:133:LEU:HD23 | 1.81 | 0.41 |
| 5:HB:89:TYR:CZ | 5:HB:139:ALA:HA | 2.56 | 0.41 |
| 5:HB:548:GLY:O | 5:HD:568:LYS:HB3 | 2.21 | 0.41 |
| 5:HB:584:THR:O | 5:HC:531:ASN:ND2 | 2.44 | 0.41 |
| 5:HC:320:LEU:HB3 | 5:HC:358:VAL:HB | 2.03 | 0.41 |
| 5:HC:492:GLU:O | 5:HC:514:HIS:HE1 | 2.04 | 0.41 |
| 5:HC:56:SER:OG | 5:HC:57:GLY:N | 2.54 | 0.41 |
| 5:HD:104:VAL:HG22 | 5:HD:105:ASN:N | 2.35 | 0.41 |
| 6:HF:86:ASP:CG | 6:HF:180:GLN:HE21 | 2.18 | 0.41 |
| 7:HH:75:ALA:HB1 | 7:HI:75:ALA:HB1 | 2.03 | 0.41 |
| 7:HI:343:VAL:HG13 | 7:HI:524:LYS:O | 2.21 | 0.41 |
| 7:HJ:166:GLN:O | 7:HJ:170:ILE:HB | 2.20 | 0.41 |
| 7:HH:346:ILE:O | 7:HJ:348:MET:HB2 | 2.21 | 0.41 |
| 7:HJ:405:ARG:HB2 | 7:HJ:430:THR:OG1 | 2.20 | 0.41 |
| 5:I:139:ALA:C | 5:I:141:GLY:H | 2.23 | 0.41 |
| 5:I:322:GLY:N | 5:I:360:THR:HG23 | 2.35 | 0.41 |
| 8:IB:49:ILE:HG23 | 8:IB:60:VAL:O | 2.21 | 0.41 |
| 11:IE:174:LYS:O | 11:IE:177:ILE:HG22 | 2.21 | 0.41 |
| 11:IE:23:ILE:HG22 | 11:IE:24:PRO:O | 2.21 | 0.41 |
| 5:K:118:LYS:HA | 5:K:142:ARG:CZ | 2.51 | 0.41 |
| 5:K:177:PHE:O | 5:K:230:ILE:HG13 | 2.20 | 0.41 |
| 5:J:326:MET:CE | 5:K:264:ARG:HB3 | 2.51 | 0.41 |
| 6:L:79:PRO:HD2 | 6:L:193:TRP:CB | 2.51 | 0.41 |
| 6:N:13:ARG:HG2 | 6:N:14:LEU:N | 2.27 | 0.41 |
| 7:O:216:MET:HG3 | 7:O:217:ASN:N | 2.36 | 0.41 |
| 7:O:501:THR:HB | 7:Q:422:LYS:NZ | 2.36 | 0.41 |
| 7:O:85:LEU:O | 7:O:88:PRO:HD2 | 2.21 | 0.41 |
| 7:Q:425:LEU:HA | 7:Q:425:LEU:HD23 | 1.82 | 0.41 |
| 8:R:49:ILE:HG23 | 8:R:60:VAL:O | 2.21 | 0.41 |
| 8:S:69:TRP:HB2 | 8:S:159:LEU:HD23 | 2.03 | 0.41 |
| 10:U:213:PRO:HG3 | 10:U:219:LEU:HD12 | 2.03 | 0.41 |
| 11:V:166:LEU:HA | 11:V:166:LEU:HD23 | 1.83 | 0.41 |
| 11:V:186:ARG:CG | 11:V:187:ILE:H | 2.34 | 0.41 |
| 12:W:99:SER:HB3 | 12:W:102:GLY:H | 1.84 | 0.41 |
| 1:X:278:ALA:HB2 | 1:X:317:GLY:N | 2.33 | 0.41 |
| 1:X:302:GLU:HG2 | 1:X:303:ASN:N | 2.36 | 0.41 |
| 1:X:278:ALA:H | 1:X:316:GLY:HA2 | 1.85 | 0.41 |
| 1:X:23:GLY:HA2 | 1:X:68:GLN:NE2 | 2.35 | 0.41 |
| 1:Y:220:THR:HA | 1:Y:260:LEU:HD13 | 2.03 | 0.41 |
| 1:Y:394:ASN:O | 1:Y:397:LYS:HG2 | 2.21 | 0.41 |
| 1:Y:565:GLU:OE1 | 1:Y:571:PRO:HD3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:66:TYR:O | 1:Y:69:GLN:N | 2.54 | 0.41 |
| 13:YA:148[A]:GLN:HG3 | 13:YA:421[A]:TYR:CE1 | 2.56 | 0.41 |
| 13:YA:463[A]:ILE:O | 13:YB:455[A]:LYS:HA | 2.21 | 0.41 |
| 13:YA:553[B]:LYS:HA | 13:YC:560[B]:ILE:O | 2.21 | 0.41 |
| 13:YB:116[D]:ASP:OD2 | 13:YB:121[D]:TYR:N | 2.43 | 0.41 |
| 13:YB:148[D]:GLN:HG3 | 13:YB:421[D]:TYR:CE1 | 2.56 | 0.41 |
| 13:YB:148[E]:GLN:HG3 | 13:YB:421[E]:TYR:CE1 | 2.56 | 0.41 |
| 13:YB:227[D]:ARG:HG2 | 13:YB:228[D]:GLU:N | 2.36 | 0.41 |
| 13:YB:418[F]:THR:HG21 | 13:YC:428[F]:GLY:CA | 2.49 | 0.41 |
| 13:YB:450[C]:VAL:HG11 | 13:YC:446[C]:GLY:H | 1.85 | 0.41 |
| 13:YB:453[F]:ASP:O | 13:YC:445[F]:ASP:HA | 2.20 | 0.41 |
| 13:YB:468[F]:ASP:HB3 | 13:YC:461[F]:SER:CA | 2.51 | 0.41 |
| 13:YB:506[E]:VAL:HA | 13:YC:498[E]:VAL:O | 2.21 | 0.41 |
| 13:YB:61[F]:ILE:CG2 | 13:YC:59[F]:GLN:HA | 2.51 | 0.41 |
| 13:YB:61[D]:ILE:HG13 | 13:YB:62[D]:THR:N | 2.34 | 0.41 |
| 13:YA:61[E]:ILE:O | 13:YB:75[E]:GLY:O | 2.39 | 0.41 |
| 13:YC:148[B]:GLN:HG3 | 13:YC:421[B]:TYR:CE1 | 2.56 | 0.41 |
| 13:YC:227[B]:ARG:HG2 | 13:YC:228[B]:GLU:N | 2.36 | 0.41 |
| 13:YC:227[D]:ARG:HG2 | 13:YC:228[D]:GLU:N | 2.36 | 0.41 |
| 13:YC:293[C]:ASN:HA | 13:YC:296[C]:LEU:HB2 | 2.02 | 0.41 |
| 13:YC:336[F]:LEU:HA | 13:YC:336[F]:LEU:HD12 | 1.84 | 0.41 |
| 13:YC:38[A]:GLN:O | 13:YC:46[A]:GLY:HA2 | 2.20 | 0.41 |
| 13:YC:16[C]:GLU:OE2 | 13:YC:49[C]:THR:OG1 | 2.39 | 0.41 |
| 13:YA:561[A]:SER:O | 13:YC:569[A]:GLY:HA2 | 2.21 | 0.41 |
| 13:YC:8[B]:LEU:HD23 | 13:YC:8[B]:LEU:HA | 1.79 | 0.41 |
| 14:YD:114[D]:SER:HA | 14:YD:167[D]:GLU:OE1 | 2.20 | 0.41 |
| 13:YA:47[E]:ILE:HG12 | 14:YD:123[E]:PRO:HD3 | 2.02 | 0.41 |
| 14:YD:210[C]:PRO:HB2 | 14:YD:228[C]:TYR:CD2 | 2.56 | 0.41 |
| 14:YD:290[C]:ASN:O | 14:YD:292[C]:TYR:N | 2.54 | 0.41 |
| 14:YD:345[C]:GLU:HB3 | 14:YD:352[C]:VAL:HG13 | 2.03 | 0.41 |
| 14:YE:51[E]:MET:SD | 14:YE:108[E]:GLU:HA | 2.61 | 0.41 |
| 14:YE:114[B]:SER:HA | 14:YE:167[B]:GLU:OE1 | 2.20 | 0.41 |
| 14:YE:124[A]:PHE:CZ | 14:YE:135[A]:MET:HG2 | 2.56 | 0.41 |
| 14:YE:279[A]:ARG:HD3 | 14:YE:279[A]:ARG:HA | 1.43 | 0.41 |
| 14:YE:16[A]:LEU:CD2 | 14:YE:29[A]:VAL:HB | 2.51 | 0.41 |
| 14:YE:47[F]:ARG:NH1 | 14:YE:341[F]:GLU:OE1 | 2.54 | 0.41 |
| 14:YE:360[C]:ASN:ND2 | 14:YE:360[C]:ASN:N | 2.68 | 0.41 |
| 14:YF:124[F]:PHE:CZ | 14:YF:135[F]:MET:HG2 | 2.56 | 0.41 |
| 14:YF:136[E]:LEU:HD21 | 14:YF:166[E]:PHE:CE2 | 2.56 | 0.41 |
| 14:YF:210[A]:PRO:HB2 | 14:YF:228[A]:TYR:CD2 | 2.55 | 0.41 |
| 10:ID:286:VAL:H | 14:YF:215[B]:GLU:CD | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YF:210[D]:PRO:HB2 | 14:YF:228[D]:TYR:CD2 | 2.56 | 0.41 |
| 14:YF:334[E]:LYS:HA | 14:YF:334[E]:LYS:HD2 | 1.93 | 0.41 |
| 14:YF:345[F]:GLU:HB3 | 14:YF:352[F]:VAL:HG13 | 2.03 | 0.41 |
| 2:Z:146:LEU:HA | 2:Z:585:MET:HA | 2.02 | 0.41 |
| 2:Z:379:ILE:HD11 | 2:Z:402:GLY:H | 1.86 | 0.41 |
| 2:Z:442:SER:HA | 2:Z:491:ILE:HD13 | 2.03 | 0.41 |
| 2:Z:752:TYR:O | 2:Z:753:ASN:OD1 | 2.39 | 0.41 |
| 2:Z:821:ILE:N | 2:Z:824:GLN:NE2 | 2.69 | 0.41 |
| 2:Z:861:TYR:HE2 | 2:Z:863:VAL:HG22 | 1.86 | 0.41 |
| 1:A:302:GLU:HG2 | 1:A:303:ASN:N | 2.36 | 0.41 |
| 4:AB:35:PHE:CD1 | 4:AB:39:TYR:HE2 | 2.39 | 0.41 |
| 5:AC:104:VAL:HG22 | 5:AC:105:ASN:H | 1.86 | 0.41 |
| 5:AC:382:ASN:O | 5:AC:383:ILE:HD13 | 2.20 | 0.41 |
| 5:AC:590:GLN:OE1 | 5:AD:589:ILE:HA | 2.21 | 0.41 |
| 5:AC:67:SER:HA | 5:AC:94:ARG:O | 2.20 | 0.41 |
| 5:AD:94:ARG:CD | 5:AD:134:GLU:HG2 | 2.51 | 0.41 |
| 5:AD:144:GLU:OE1 | 5:AD:144:GLU:N | 2.54 | 0.41 |
| 5:AC:264:ARG:HD3 | 5:AE:327:PRO:HG3 | 2.03 | 0.41 |
| 5:AC:550:VAL:N | 5:AE:569:TYR:O | 2.50 | 0.41 |
| 6:AF:135:GLU:O | 6:AF:139:SER:N | 2.26 | 0.41 |
| 6:AG:88:TRP:HB3 | 6:AG:90:PHE:CE1 | 2.55 | 0.41 |
| 7:AI:197:ALA:O | 7:AI:201:GLN:HG3 | 2.20 | 0.41 |
| 7:AJ:433:TYR:CE2 | 7:AJ:436:GLU:HB2 | 2.56 | 0.41 |
| 1:B:347:THR:OG1 | 1:B:348:PHE:N | 2.54 | 0.41 |
| 1:B:378:PRO:HG2 | 1:B:381:GLY:O | 2.21 | 0.41 |
| 12:BG:113:PHE:CE1 | 12:BG:170:ASN:HA | 2.56 | 0.41 |
| 1:BH:243:ILE:HG22 | 1:BH:258:GLY:HA3 | 2.03 | 0.41 |
| 1:BH:360:VAL:HG23 | 1:BH:375:ALA:O | 2.21 | 0.41 |
| 1:BH:59:LEU:CD1 | 1:BI:37:LEU:HD12 | 2.51 | 0.41 |
| 1:BH:657:PRO:O | 1:BH:658:ILE:HD13 | 2.21 | 0.41 |
| 1:BI:145:PHE:CD1 | 1:BI:169:GLN:HA | 2.56 | 0.41 |
| 1:BI:537:ASP:OD1 | 1:BI:537:ASP:N | 2.46 | 0.41 |
| 2:BJ:206:GLN:C | 2:BJ:208:VAL:N | 2.75 | 0.41 |
| 2:BJ:28:VAL:HG23 | 2:BJ:29:GLY:N | 2.35 | 0.41 |
| 2:BJ:300:LEU:N | 2:BJ:301:PRO:CD | 2.84 | 0.41 |
| 2:BJ:380:ILE:HB | 2:BJ:396:ILE:HG21 | 2.01 | 0.41 |
| 2:BJ:412:THR:OG1 | 2:BJ:413:TRP:N | 2.53 | 0.41 |
| 2:BJ:6:PRO:O | 2:BJ:7:SER:OG | 2.27 | 0.41 |
| 2:BJ:793:CYS:HB3 | 2:BJ:813:ILE:HG21 | 2.03 | 0.41 |
| 2:BJ:969:TYR:OH | 5:CH:18:TYR:CZ | 2.68 | 0.41 |
| 2:C:228:ARG:HD2 | 5:K:556:GLN:NE2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:251:ASP:OD2 | 2:C:252:LYS:HG3 | 2.20 | 0.41 |
| 2:C:319:TYR:CD2 | 2:C:375:VAL:HG21 | 2.56 | 0.41 |
| 2:C:793:CYS:HB3 | 2:C:813:ILE:HG21 | 2.03 | 0.41 |
| 3:CB:154:LEU:HA | 3:CB:154:LEU:HD23 | 1.86 | 0.41 |
| 4:CC:15:ILE:HD13 | 4:CE:25:PHE:HB2 | 2.02 | 0.41 |
| 5:CF:81:LEU:HD22 | 5:CF:143:TRP:CZ3 | 2.56 | 0.41 |
| 5:CF:30:PHE:O | 5:CF:33:LEU:HG | 2.21 | 0.41 |
| 5:CG:258:TYR:HA | 5:CG:385:TRP:O | 2.21 | 0.41 |
| 5:CH:304:ILE:HG23 | 5:CH:385:TRP:CD1 | 2.56 | 0.41 |
| 5:CH:433:VAL:HG12 | 5:CH:434:GLU:N | 2.36 | 0.41 |
| 6:CJ:88:TRP:HB3 | 6:CJ:90:PHE:CE1 | 2.55 | 0.41 |
| 3:D:310:ILE:HG13 | 3:D:311:TYR:N | 2.36 | 0.41 |
| 7:DB:451:PHE:CE1 | 7:DB:470:GLY:HA2 | 2.56 | 0.41 |
| 7:DB:192:GLN:HG3 | 7:DC:188:GLN:CD | 2.41 | 0.41 |
| 7:DC:283:TRP:CZ3 | 7:DC:284:ASN:HB3 | 2.55 | 0.41 |
| 7:DC:433:TYR:CE2 | 7:DC:436:GLU:HB2 | 2.56 | 0.41 |
| 7:DC:335:ASN:N | 7:DD:329:ASN:HD21 | 2.19 | 0.41 |
| 8:DE:121:LYS:HG2 | 8:DE:122:THR:N | 2.36 | 0.41 |
| 11:DI:107:ASP:HA | 11:DI:155:THR:CG2 | 2.51 | 0.41 |
| 3:E:104:TYR:CB | 3:E:165:ARG:HB2 | 2.49 | 0.41 |
| 3:E:80:LYS:HG2 | 3:E:81:VAL:H | 1.85 | 0.41 |
| 1:EA:527:ASP:C | 1:EA:527:ASP:OD1 | 2.60 | 0.41 |
| 1:EA:55:VAL:O | 1:EA:58:ASP:HB3 | 2.20 | 0.41 |
| 1:EB:167:LEU:HD23 | 1:EB:167:LEU:HA | 1.84 | 0.41 |
| 2:EC:217:GLN:HG2 | 2:EC:218:THR:N | 2.36 | 0.41 |
| 2:EC:589:LYS:HD2 | 2:EC:590:ALA:H | 1.86 | 0.41 |
| 2:EC:793:CYS:HB3 | 2:EC:813:ILE:HG21 | 2.03 | 0.41 |
| 2:EC:958:MET:O | 2:EC:961:VAL:HG23 | 2.21 | 0.41 |
| 3:ED:282:LYS:NZ | 3:ED:287:ASP:O | 2.53 | 0.41 |
| 4:EF:4:GLN:OE1 | 4:EH:61:ILE:HB | 2.21 | 0.41 |
| 5:EI:89:TYR:CZ | 5:EI:139:ALA:HA | 2.56 | 0.41 |
| 5:EI:139:ALA:C | 5:EI:141:GLY:H | 2.23 | 0.41 |
| 5:EI:304:ILE:HD12 | 5:EI:384:THR:O | 2.21 | 0.41 |
| 5:EI:560:ASP:HB3 | 5:EI:561:GLU:H | 1.66 | 0.41 |
| 5:EJ:229:ASN:OD1 | 5:EJ:230:ILE:N | 2.54 | 0.41 |
| 5:EJ:258:TYR:HA | 5:EJ:385:TRP:O | 2.21 | 0.41 |
| 5:EJ:344:VAL:O | 5:EJ:345:LEU:HD12 | 2.20 | 0.41 |
| 4:F:50:VAL:O | 4:F:52:ASN:N | 2.54 | 0.41 |
| 5:FA:326:MET:HE3 | 5:FA:326:MET:HB2 | 1.81 | 0.41 |
| 6:FC:70:ILE:HD12 | 6:FC:196:LEU:HD11 | 2.03 | 0.41 |
| 7:FE:12:GLU:CG | 7:FE:15:TYR:H | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:232:THR:HG23 | 7:FE:234:SER:N | 2.37 | 0.41 |
| 7:FE:251:ASN:OD1 | 7:FF:260:ARG:HB2 | 2.21 | 0.41 |
| 7:FE:304:ASP:HB3 | 7:FG:299:THR:HG22 | 2.03 | 0.41 |
| 7:FE:77:THR:HG23 | 7:FE:79:ALA:H | 1.85 | 0.41 |
| 7:FF:17:LYS:HD2 | 7:FF:18:PHE:H | 1.86 | 0.41 |
| 7:FG:99:ARG:O | 7:FG:114:SER:HA | 2.21 | 0.41 |
| 7:FF:315:ILE:O | 7:FG:321:MET:HA | 2.21 | 0.41 |
| 7:FE:346:ILE:HB | 7:FG:348:MET:HB2 | 2.03 | 0.41 |
| 7:FG:32:VAL:O | 7:FG:36:ILE:HG12 | 2.20 | 0.41 |
| 8:FI:61:ALA:HB2 | 8:IB:133:TRP:CH2 | 2.55 | 0.41 |
| 1:EA:52:ARG:CZ | 9:FJ:25:ARG:HD2 | 2.50 | 0.41 |
| 4:G:213:LYS:HE3 | 4:G:249:ILE:HG12 | 2.03 | 0.41 |
| 12:GC:15:ASP:CG | 12:GC:16:PHE:N | 2.71 | 0.41 |
| 12:GC:30:PRO:HG2 | 12:GC:177:TRP:HE1 | 1.86 | 0.41 |
| 1:GE:240:GLU:HG2 | 1:GE:240:GLU:O | 2.21 | 0.41 |
| 1:GE:414:LEU:O | 1:GE:415:PHE:HD1 | 2.04 | 0.41 |
| 2:GF:1012:LEU:O | 2:GF:1012:LEU:HD12 | 2.21 | 0.41 |
| 2:GF:451:LEU:HD12 | 2:GF:452:SER:N | 2.36 | 0.41 |
| 2:GF:541:TYR:CG | 2:GF:542:THR:N | 2.85 | 0.41 |
| 2:GF:589:LYS:HD2 | 2:GF:590:ALA:H | 1.86 | 0.41 |
| 4:GI:44:ASP:O | 4:GI:59:GLN:NE2 | 2.52 | 0.41 |
| 5:HB:313:PHE:CD2 | 5:HB:320:LEU:HD21 | 2.56 | 0.41 |
| 5:HC:338:ASP:HB3 | 5:HC:349:TRP:CD1 | 2.56 | 0.41 |
| 5:HC:532:LEU:HD23 | 5:HC:532:LEU:HA | 1.87 | 0.41 |
| 5:HD:399:ILE:O | 5:HD:402:GLU:HB3 | 2.20 | 0.41 |
| 5:HD:97:ASP:OD1 | 5:HD:102:TRP:CE2 | 2.74 | 0.41 |
| 6:HG:126:VAL:HG13 | 6:HG:156:LEU:HD11 | 2.03 | 0.41 |
| 7:HH:12:GLU:CG | 7:HH:15:TYR:H | 2.34 | 0.41 |
| 7:HH:85:LEU:O | 7:HH:88:PRO:HD2 | 2.21 | 0.41 |
| 7:HI:479:ASN:HB2 | 7:HJ:469:VAL:O | 2.21 | 0.41 |
| 7:HI:491:ASP:HB2 | 7:HI:496:ARG:CG | 2.51 | 0.41 |
| 5:I:560:ASP:HB3 | 5:I:561:GLU:H | 1.66 | 0.41 |
| 5:I:67:SER:HA | 5:I:94:ARG:O | 2.20 | 0.41 |
| 11:IE:160:VAL:O | 11:IE:164:GLU:N | 2.54 | 0.41 |
| 5:J:304:ILE:CD1 | 5:J:385:TRP:HA | 2.40 | 0.41 |
| 5:J:49:TRP:CD1 | 5:J:49:TRP:N | 2.87 | 0.41 |
| 5:K:95:ALA:HB3 | 5:K:133:LEU:HB2 | 2.03 | 0.41 |
| 5:K:213:GLY:HA2 | 5:K:221:GLU:HB2 | 2.02 | 0.41 |
| 5:K:192:ARG:CG | 5:K:245:GLU:HB2 | 2.50 | 0.41 |
| 6:M:26:ASP:HB3 | 6:M:34:SER:HA | 2.03 | 0.41 |
| 7:O:12:GLU:CG | 7:O:15:TYR:H | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:503:ASN:ND2 | 7:Q:446:LYS:H | 2.19 | 0.41 |
| 7:P:240:ASN:HB3 | 7:P:243:VAL:HG22 | 2.03 | 0.41 |
| 7:P:250:LEU:HD23 | 7:Q:253:ARG:HH11 | 1.86 | 0.41 |
| 7:Q:453:GLU:HG3 | 7:Q:475:LEU:HD21 | 2.02 | 0.41 |
| 8:S:142:LEU:HD21 | 8:IB:21:PHE:CG | 2.56 | 0.41 |
| 1:A:52:ARG:CZ | 9:T:25:ARG:HD2 | 2.51 | 0.41 |
| 11:V:174:LYS:O | 11:V:177:ILE:HG22 | 2.21 | 0.41 |
| 11:V:6:PHE:HE1 | 11:V:188:MET:O | 2.03 | 0.41 |
| 1:X:222:THR:O | 1:X:223:ILE:HG12 | 2.21 | 0.41 |
| 1:X:243:ILE:HG22 | 1:X:258:GLY:HA3 | 2.03 | 0.41 |
| 1:X:277:GLY:O | 1:X:279:ASP:N | 2.50 | 0.41 |
| 1:X:572:TYR:CE2 | 1:X:574:GLY:HA3 | 2.55 | 0.41 |
| 1:X:611:LEU:HD23 | 1:X:611:LEU:HA | 1.82 | 0.41 |
| 1:X:657:PRO:O | 1:X:658:ILE:HD13 | 2.21 | 0.41 |
| 13:YA:336[D]:LEU:HA | 13:YA:336[D]:LEU:HD12 | 1.85 | 0.41 |
| 13:YA:552[D]:GLU:CG | 13:YA:554[D]:MET:HE1 | 2.51 | 0.41 |
| 13:YA:318[D]:GLN:NE2 | 13:YB:367[D]:PRO:HB2 | 2.36 | 0.41 |
| 13:YB:506[E]:VAL:HG21 | 13:YC:502[E]:VAL:HG21 | 2.02 | 0.41 |
| 13:YB:83[E]:TYR:OH | 13:YB:85[E]:HIS:HE1 | 2.04 | 0.41 |
| 13:YC:266[C]:TRP:NE1 | 13:YC:274[C]:GLN:HG2 | 2.36 | 0.41 |
| 13:YC:266[F]:TRP:NE1 | 13:YC:274[F]:GLN:HG2 | 2.36 | 0.41 |
| 13:YC:336[D]:LEU:HD12 | 13:YC:336[D]:LEU:HA | 1.85 | 0.41 |
| 13:YC:399[F]:HIS:ND1 | 13:YC:417[F]:PRO:HD3 | 2.36 | 0.41 |
| 13:YC:76[D]:PRO:HB2 | 13:YC:98[D]:GLY:CA | 2.51 | 0.41 |
| 14:YD:170[A]:LEU:HA | 14:YD:170[A]:LEU:HD23 | 1.69 | 0.41 |
| 14:YD:170[D]:LEU:HD23 | 14:YD:170[D]:LEU:HA | 1.68 | 0.41 |
| 14:YD:212[C]:ILE:HG12 | 14:YD:228[C]:TYR:HB2 | 2.03 | 0.41 |
| 14:YD:290[A]:ASN:O | 14:YD:292[A]:TYR:N | 2.54 | 0.41 |
| 14:YD:290[D]:ASN:C | 14:YD:290[D]:ASN:OD1 | 2.58 | 0.41 |
| 14:YD:345[A]:GLU:HB3 | 14:YD:352[A]:VAL:HG13 | 2.03 | 0.41 |
| 14:YD:345[F]:GLU:HB3 | 14:YD:352[F]:VAL:HG13 | 2.03 | 0.41 |
| 14:YD:44[A]:LEU:HD23 | 14:YD:44[A]:LEU:HA | 1.85 | 0.41 |
| 14:YE:174[B]:ARG:HG3 | 14:YE:188[B]:VAL:HG22 | 2.03 | 0.41 |
| 14:YE:230[D]:LEU:HD13 | 14:YE:230[D]:LEU:HA | 1.85 | 0.41 |
| 14:YE:259[D]:LEU:HD23 | 14:YE:259[D]:LEU:HA | 1.83 | 0.41 |
| 14:YE:290[E]:ASN:O | 14:YE:292[E]:TYR:N | 2.54 | 0.41 |
| 11:GB:175:SER:HA | 14:YF:217[A]:SER:HB2 | 2.02 | 0.41 |
| 14:YF:290[F]:ASN:OD1 | 14:YF:290[F]:ASN:C | 2.58 | 0.41 |
| 2:Z:307:ILE:HG22 | 2:Z:308:ALA:N | 2.36 | 0.41 |
| 2:Z:31:ASN:O | 2:Z:32:PHE:HD1 | 2.04 | 0.41 |
| 2:Z:472:LYS:HG3 | 2:Z:474:GLU:HG3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:484:HIS:O | 2:Z:485:TYR:HB3 | 2.21 | 0.41 |
| 2:Z:577:GLY:N | 2:Z:606:ASP:O | 2.54 | 0.41 |
| 2:Z:627:GLU:HB2 | 2:Z:628:HIS:CD2 | 2.56 | 0.41 |
| 2:Z:788:THR:OG1 | 2:Z:789:ALA:N | 2.54 | 0.41 |
| 15:ZA:56[F]:HIS:CD2 | 15:ZA:83[F]:CYS:HB2 | 2.56 | 0.41 |
| 1:A:108:THR:OG1 | 1:A:109:GLU:N | 2.54 | 0.40 |
| 1:A:201:VAL:HG21 | 1:A:262:PRO:HB3 | 2.02 | 0.40 |
| 4:AA:50:VAL:O | 4:AA:52:ASN:N | 2.54 | 0.40 |
| 5:AC:289:LYS:HG3 | 5:AC:370:HIS:CE1 | 2.56 | 0.40 |
| 5:AE:95:ALA:HB3 | 5:AE:133:LEU:HB2 | 2.03 | 0.40 |
| 6:AF:26:ASP:HB3 | 6:AF:34:SER:HA | 2.03 | 0.40 |
| 6:AG:201:VAL:N | 6:AG:210:THR:O | 2.31 | 0.40 |
| 6:AG:79:PRO:HD2 | 6:AG:193:TRP:CB | 2.51 | 0.40 |
| 6:AH:195:LEU:HA | 6:AH:215:PHE:HD1 | 1.85 | 0.40 |
| 7:AI:12:GLU:CG | 7:AI:15:TYR:H | 2.34 | 0.40 |
| 7:AJ:424:ARG:O | 7:BA:504:ARG:NH2 | 2.35 | 0.40 |
| 7:AJ:453:GLU:HG3 | 7:AJ:475:LEU:HD11 | 2.03 | 0.40 |
| 7:AJ:491:ASP:HB2 | 7:AJ:496:ARG:CG | 2.51 | 0.40 |
| 1:B:515:PHE:O | 1:B:537:ASP:HA | 2.22 | 0.40 |
| 7:BA:196:VAL:CG2 | 7:BA:214:THR:HG22 | 2.52 | 0.40 |
| 7:BA:351:ALA:O | 7:BA:520:ASN:ND2 | 2.54 | 0.40 |
| 7:BA:453:GLU:HG3 | 7:BA:475:LEU:HD21 | 2.02 | 0.40 |
| 7:AI:439:ILE:HG12 | 7:BA:515:TRP:CZ3 | 2.56 | 0.40 |
| 8:BB:121:LYS:HG2 | 8:BB:122:THR:N | 2.37 | 0.40 |
| 8:BB:118:ARG:HE | 8:BC:62:GLY:HA2 | 1.84 | 0.40 |
| 10:BE:221:ALA:O | 10:BE:225:ILE:N | 2.46 | 0.40 |
| 12:BG:15:ASP:CG | 12:BG:16:PHE:N | 2.71 | 0.40 |
| 12:BG:124:MET:HG3 | 12:BG:170:ASN:ND2 | 2.35 | 0.40 |
| 12:BG:196:GLU:HG2 | 12:BG:218:MET:O | 2.21 | 0.40 |
| 1:BH:222:THR:O | 1:BH:223:ILE:HG12 | 2.21 | 0.40 |
| 1:BH:99:LEU:O | 1:BH:99:LEU:HD12 | 2.21 | 0.40 |
| 1:BI:244:SER:O | 1:BI:253:THR:OG1 | 2.34 | 0.40 |
| 1:BI:236:PHE:CD2 | 1:BI:270:ILE:HD11 | 2.57 | 0.40 |
| 1:BI:352:ARG:O | 1:BI:353:PHE:HB2 | 2.21 | 0.40 |
| 1:BI:59:LEU:HD13 | 2:BJ:668:CYS:SG | 2.61 | 0.40 |
| 1:BI:66:TYR:OH | 11:DI:57:GLU:OE1 | 2.39 | 0.40 |
| 2:BJ:376:PHE:HB2 | 2:BJ:405:VAL:HA | 2.02 | 0.40 |
| 2:BJ:447:ASN:OD1 | 2:BJ:448:PHE:N | 2.54 | 0.40 |
| 2:BJ:484:HIS:O | 2:BJ:485:TYR:HB3 | 2.21 | 0.40 |
| 2:BJ:593:GLU:HB3 | 2:BJ:594:ILE:H | 1.61 | 0.40 |
| 2:C:300:LEU:N | 2:C:301:PRO:CD | 2.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:379:ILE:HD11 | 2:C:402:GLY:H | 1.86 | 0.40 |
| 2:C:376:PHE:CZ | 2:C:441:VAL:HG11 | 2.51 | 0.40 |
| 2:C:451:LEU:HD12 | 2:C:452:SER:N | 2.36 | 0.40 |
| 2:C:115:GLU:HB2 | 2:C:598:TYR:CE1 | 2.56 | 0.40 |
| 2:C:976:SER:C | 2:C:977:ILE:HG13 | 2.40 | 0.40 |
| 3:CA:255:SER:O | 3:CA:258:PHE:N | 2.53 | 0.40 |
| 3:CB:115:ASN:HA | 3:CB:121:ALA:HA | 2.02 | 0.40 |
| 4:CD:35:PHE:CD1 | 4:CD:39:TYR:HE2 | 2.40 | 0.40 |
| 5:CG:104:VAL:HG13 | 5:CG:105:ASN:H | 1.85 | 0.40 |
| 5:CG:144:GLU:N | 5:CG:144:GLU:OE1 | 2.54 | 0.40 |
| 5:CG:326:MET:CE | 5:CH:264:ARG:HB3 | 2.51 | 0.40 |
| 5:CG:338:ASP:HB3 | 5:CG:349:TRP:CD1 | 2.56 | 0.40 |
| 5:CF:542:LEU:HD21 | 5:CG:569:TYR:CZ | 2.56 | 0.40 |
| 5:CH:153:LYS:HG3 | 5:CH:153:LYS:O | 2.21 | 0.40 |
| 3:D:248:ARG:HA | 3:D:330:ILE:O | 2.20 | 0.40 |
| 6:DA:200:THR:HA | 6:DA:211:VAL:HA | 2.03 | 0.40 |
| 7:DB:12:GLU:CG | 7:DB:15:TYR:H | 2.34 | 0.40 |
| 7:DB:171:LYS:HA | 7:DB:174:ALA:HB3 | 2.03 | 0.40 |
| 7:DC:343:VAL:O | 7:DC:378:ARG:NH1 | 2.49 | 0.40 |
| 8:DF:121:LYS:HG2 | 8:DF:122:THR:N | 2.37 | 0.40 |
| 10:DH:213:PRO:HG3 | 10:DH:219:LEU:HD12 | 2.03 | 0.40 |
| 11:DI:6:PHE:HE1 | 11:DI:188:MET:O | 2.03 | 0.40 |
| 12:DJ:196:GLU:HG2 | 12:DJ:218:MET:O | 2.21 | 0.40 |
| 1:EB:145:PHE:CD1 | 1:EB:169:GLN:HA | 2.56 | 0.40 |
| 1:EB:22:VAL:HG12 | 1:EB:23:GLY:N | 2.36 | 0.40 |
| 2:EC:376:PHE:HB2 | 2:EC:405:VAL:HA | 2.02 | 0.40 |
| 2:EC:690:ILE:HD12 | 2:EC:690:ILE:HA | 1.87 | 0.40 |
| 2:EC:899:PHE:O | 2:EC:900:ILE:HD13 | 2.21 | 0.40 |
| 2:EC:904:LEU:HD12 | 2:EC:905:THR:N | 2.36 | 0.40 |
| 3:ED:95:TRP:CZ2 | 3:ED:169:PRO:HD3 | 2.55 | 0.40 |
| 3:EE:149:ASP:OD1 | 3:EE:150:LYS:N | 2.54 | 0.40 |
| 3:EE:210:VAL:HG13 | 3:EE:211:PRO:HD2 | 2.02 | 0.40 |
| 4:EF:149:ARG:HB3 | 4:EH:168:PHE:CZ | 2.56 | 0.40 |
| 4:EG:35:PHE:CD1 | 4:EG:39:TYR:HE2 | 2.39 | 0.40 |
| 4:EG:61:ILE:O | 4:EH:4:GLN:NE2 | 2.50 | 0.40 |
| 5:EI:166:GLU:HB2 | 5:FA:201:TYR:CD2 | 2.56 | 0.40 |
| 5:EJ:304:ILE:CD1 | 5:EJ:385:TRP:HA | 2.40 | 0.40 |
| 5:EI:1:MET:H2 | 5:EJ:41:ASP:HB3 | 1.86 | 0.40 |
| 5:EJ:460:TYR:OH | 5:EJ:462:ASN:HB2 | 2.22 | 0.40 |
| 5:FA:321:ALA:O | 5:FA:324:VAL:HG12 | 2.22 | 0.40 |
| 5:FA:433:VAL:HG12 | 5:FA:434:GLU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:FE:130:GLU:OE2 | 7:FF:132:ARG:NH1 | 2.40 | 0.40 |
| 7:FE:161:THR:H | 7:FE:164:LYS:HZ1 | 1.69 | 0.40 |
| 7:FE:160:MET:HG2 | 7:FE:165:THR:HB | 2.03 | 0.40 |
| 7:FE:216:MET:HG3 | 7:FE:217:ASN:N | 2.36 | 0.40 |
| 7:FE:227:VAL:HG23 | 7:FF:225:LYS:HB3 | 2.03 | 0.40 |
| 7:FE:451:PHE:CE1 | 7:FE:470:GLY:HA2 | 2.56 | 0.40 |
| 7:FE:470:GLY:O | 7:FG:476:ASP:N | 2.51 | 0.40 |
| 7:FF:223:GLU:HG3 | 7:FF:224:TYR:CE1 | 2.57 | 0.40 |
| 7:FF:240:ASN:HB3 | 7:FF:243:VAL:HG22 | 2.03 | 0.40 |
| 7:FE:97:LEU:HD22 | 7:FF:96:GLY:HA2 | 2.02 | 0.40 |
| 8:FH:32:PHE:O | 8:FH:35:GLN:N | 2.50 | 0.40 |
| 8:FH:69:TRP:HB2 | 8:FH:159:LEU:HD23 | 2.03 | 0.40 |
| 10:GA:213:PRO:HG3 | 10:GA:219:LEU:HD12 | 2.03 | 0.40 |
| 11:GB:174:LYS:O | 11:GB:177:ILE:HG22 | 2.21 | 0.40 |
| 11:GB:23:ILE:HG22 | 11:GB:24:PRO:O | 2.21 | 0.40 |
| 11:GB:36:PHE:CD1 | 11:GB:180:PHE:HZ | 2.39 | 0.40 |
| 1:GD:355:SER:O | 1:GD:379:LYS:HD3 | 2.21 | 0.40 |
| 1:GE:236:PHE:CD2 | 1:GE:270:ILE:HD11 | 2.57 | 0.40 |
| 2:EC:613:LYS:HB3 | 1:GE:619:GLN:HE22 | 1.85 | 0.40 |
| 1:GE:88:SER:O | 1:GE:91:GLN:HB3 | 2.21 | 0.40 |
| 2:GF:217:GLN:HG2 | 2:GF:218:THR:H | 1.85 | 0.40 |
| 2:GF:217:GLN:HG2 | 2:GF:218:THR:N | 2.36 | 0.40 |
| 2:GF:223:LYS:C | 2:GF:225:PHE:H | 2.25 | 0.40 |
| 2:GF:319:TYR:CD2 | 2:GF:375:VAL:HG21 | 2.56 | 0.40 |
| 2:GF:115:GLU:HB2 | 2:GF:598:TYR:CE1 | 2.56 | 0.40 |
| 2:GF:760:ILE:HD12 | 2:GF:760:ILE:HA | 1.90 | 0.40 |
| 2:GF:855:ILE:HD12 | 2:GF:855:ILE:HA | 1.86 | 0.40 |
| 3:GH:60:TYR:HA | 3:GH:61:PRO:HD3 | 1.96 | 0.40 |
| 4:GI:147:THR:HB | 4:GI:163:SER:OG | 2.22 | 0.40 |
| 4:HA:50:VAL:O | 4:HA:52:ASN:N | 2.54 | 0.40 |
| 5:HB:128:VAL:HB | 5:HB:131:SER:OG | 2.21 | 0.40 |
| 5:HB:264:ARG:HD3 | 5:HD:327:PRO:HG3 | 2.03 | 0.40 |
| 5:HB:275:SER:OG | 5:HB:282:VAL:N | 2.52 | 0.40 |
| 5:HC:371:PHE:HZ | 5:HC:373:SER:HB3 | 1.84 | 0.40 |
| 5:HD:213:GLY:HA2 | 5:HD:221:GLU:HB2 | 2.02 | 0.40 |
| 5:HB:544:VAL:HA | 5:HD:569:TYR:CE1 | 2.57 | 0.40 |
| 5:HD:67:SER:CB | 5:HD:94:ARG:HB2 | 2.51 | 0.40 |
| 5:HD:89:TYR:C | 5:HD:91:LYS:H | 2.23 | 0.40 |
| 6:HF:11:ILE:HB | 6:HF:12:SER:H | 1.66 | 0.40 |
| 6:HG:82:VAL:HG23 | 6:HG:187:LYS:HE3 | 2.01 | 0.40 |
| 7:HH:160:MET:HG2 | 7:HH:165:THR:HB | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:HH:259:MET:HG2 | 7:HH:260:ARG:O | 2.21 | 0.40 |
| 7:HH:520:ASN:ND2 | 7:HI:434:VAL:HG21 | 2.35 | 0.40 |
| 7:HI:190:VAL:HG12 | 7:HJ:190:VAL:HG13 | 2.03 | 0.40 |
| 7:HI:320:ARG:HG2 | 7:HJ:325:TYR:HB2 | 2.04 | 0.40 |
| 5:I:304:ILE:HD12 | 5:I:384:THR:O | 2.21 | 0.40 |
| 5:I:340:VAL:HG21 | 6:M:174:TYR:N | 2.34 | 0.40 |
| 8:IA:69:TRP:HB2 | 8:IA:159:LEU:HD23 | 2.03 | 0.40 |
| 9:IC:59:ASP:O | 9:IC:63:GLU:N | 2.54 | 0.40 |
| 11:IE:9:ILE:HG12 | 11:IE:10:GLU:O | 2.21 | 0.40 |
| 5:J:253:GLN:HB2 | 5:J:255:ARG:NE | 2.37 | 0.40 |
| 5:J:320:LEU:HD23 | 5:J:358:VAL:CG2 | 2.49 | 0.40 |
| 5:I:460:TYR:CE1 | 5:J:458:THR:HG23 | 2.55 | 0.40 |
| 5:K:102:TRP:N | 5:K:102:TRP:CD1 | 2.83 | 0.40 |
| 5:K:390:LEU:HD23 | 5:K:391:GLY:N | 2.36 | 0.40 |
| 5:K:67:SER:CB | 5:K:94:ARG:HB2 | 2.51 | 0.40 |
| 6:M:144:ASN:HA | 6:M:161:LEU:HD23 | 2.04 | 0.40 |
| 7:O:134:SER:H | 7:O:142:ILE:CD1 | 2.33 | 0.40 |
| 7:O:190:VAL:HB | 7:P:189:GLY:N | 2.36 | 0.40 |
| 7:O:234:SER:HA | 5:HB:346:GLY:C | 2.42 | 0.40 |
| 7:O:276:ASP:OD1 | 7:P:260:ARG:NH2 | 2.49 | 0.40 |
| 7:O:456:ASP:CB | 7:O:462:ASN:HD21 | 2.34 | 0.40 |
| 7:P:196:VAL:HA | 7:P:199:VAL:HG22 | 2.03 | 0.40 |
| 7:P:479:ASN:HB2 | 7:Q:469:VAL:O | 2.21 | 0.40 |
| 7:O:225:LYS:HB3 | 7:Q:227:VAL:HG23 | 2.03 | 0.40 |
| 7:P:320:ARG:HG2 | 7:Q:325:TYR:HB2 | 2.03 | 0.40 |
| 9:T:58:SER:O | 9:T:62:PHE:N | 2.34 | 0.40 |
| 11:V:107:ASP:HA | 11:V:155:THR:CG2 | 2.51 | 0.40 |
| 1:X:186:ILE:O | 1:X:187:ILE:HD13 | 2.21 | 0.40 |
| 1:Y:485:VAL:HG22 | 1:Y:624:TYR:CD1 | 2.55 | 0.40 |
| 13:YA:148[F]:GLN:HG3 | 13:YA:421[F]:TYR:CE1 | 2.56 | 0.40 |
| 13:YA:180[E]:LEU:HD13 | 13:YA:180[E]:LEU:HA | 1.75 | 0.40 |
| 13:YA:227[F]:ARG:HG2 | 13:YA:228[F]:GLU:N | 2.36 | 0.40 |
| 13:YA:266[E]:TRP:NE1 | 13:YA:274[E]:GLN:HG2 | 2.36 | 0.40 |
| 13:YA:393[B]:MET:O | 13:YA:400[B]:ILE:HA | 2.21 | 0.40 |
| 13:YA:534[D]:LEU:HD11 | 13:YA:536[D]:TRP:NE1 | 2.32 | 0.40 |
| 13:YA:552[D]:GLU:HB2 | 13:YB:544[D]:TRP:HB2 | 2.03 | 0.40 |
| 13:YA:553[C]:LYS:HA | 13:YC:560[C]:ILE:O | 2.21 | 0.40 |
| 13:YA:74[B]:THR:HG21 | 13:YB:388[B]:PRO:HB2 | 2.03 | 0.40 |
| 13:YA:7[A]:ASN:OD1 | 13:YB:9[A]:ASN:ND2 | 2.54 | 0.40 |
| 13:YA:8[F]:LEU:HD23 | 13:YA:8[F]:LEU:HA | 1.80 | 0.40 |
| 13:YB:209[C]:GLN:HB3 | 13:YB:211[C]:VAL:HG23 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:277[E]:LEU:HD23 | 13:YB:277[E]:LEU:HA | 1.79 | 0.40 |
| 13:YB:321[F]:LYS:HD3 | 13:YC:452[F]:GLY:CA | 2.47 | 0.40 |
| 13:YB:399[D]:HIS:ND1 | 13:YB:417[D]:PRO:HD3 | 2.36 | 0.40 |
| 13:YB:393[F]:MET:O | 13:YB:400[F]:ILE:HA | 2.21 | 0.40 |
| 13:YB:454[B]:LYS:C | 13:YB:455[B]:LYS:HG3 | 2.40 | 0.40 |
| 13:YB:471[E]:LEU:O | 13:YC:463[E]:ILE:HA | 2.22 | 0.40 |
| 13:YB:490[B]:VAL:HG21 | 13:YC:486[B]:GLU:HB2 | 2.02 | 0.40 |
| 13:YB:490[C]:VAL:HG21 | 13:YC:486[C]:GLU:HB2 | 2.03 | 0.40 |
| 13:YB:552[B]:GLU:CB | 13:YC:544[B]:TRP:HB2 | 2.51 | 0.40 |
| 13:YA:7[C]:ASN:OD1 | 13:YB:9[C]:ASN:ND2 | 2.55 | 0.40 |
| 13:YC:148[C]:GLN:HG3 | 13:YC:421[C]:TYR:CE1 | 2.56 | 0.40 |
| 13:YC:227[C]:ARG:HG2 | 13:YC:228[C]:GLU:N | 2.36 | 0.40 |
| 13:YC:266[A]:TRP:NE1 | 13:YC:274[A]:GLN:HG2 | 2.36 | 0.40 |
| 13:YC:296[B]:LEU:HA | 13:YC:296[B]:LEU:HD12 | 1.84 | 0.40 |
| 13:YC:410[E]:GLU:O | 13:YC:426[E]:PRO:HA | 2.21 | 0.40 |
| 13:YA:438[F]:LEU:CD2 | 13:YC:442[F]:THR:HG21 | 2.47 | 0.40 |
| 13:YB:552[F]:GLU:CB | 13:YC:544[F]:TRP:HB2 | 2.51 | 0.40 |
| 13:YC:552[F]:GLU:CG | 13:YC:554[F]:MET:HE1 | 2.51 | 0.40 |
| 13:YC:76[A]:PRO:HB2 | 13:YC:98[A]:GLY:CA | 2.51 | 0.40 |
| 14:YD:136[E]:LEU:HD21 | 14:YD:166[E]:PHE:CE2 | 2.56 | 0.40 |
| 14:YD:210[D]:PRO:HB2 | 14:YD:228[D]:TYR:CD2 | 2.56 | 0.40 |
| 14:YD:210[E]:PRO:HB2 | 14:YD:228[E]:TYR:CD2 | 2.55 | 0.40 |
| 14:YD:209[B]:TYR:HB3 | 14:YD:324[B]:ILE:HG12 | 2.04 | 0.40 |
| 14:YD:360[E]:ASN:ND2 | 14:YD:360[E]:ASN:N | 2.68 | 0.40 |
| 14:YD:10[E]:PRO:HB2 | 14:YD:74[E]:VAL:HG21 | 2.04 | 0.40 |
| 14:YE:15[C]:LYS:HB3 | 14:YE:15[C]:LYS:HE2 | 1.53 | 0.40 |
| 14:YE:136[C]:LEU:HD21 | 14:YE:166[C]:PHE:CE2 | 2.56 | 0.40 |
| 13:YB:93[E]:ASN:OD1 | 14:YE:280[E]:SER:HB2 | 2.22 | 0.40 |
| 14:YE:290[F]:ASN:O | 14:YE:292[F]:TYR:N | 2.55 | 0.40 |
| 14:YE:367[A]:ILE:O | 14:YE:367[A]:ILE:HG22 | 2.21 | 0.40 |
| 14:YE:44[E]:LEU:HA | 14:YE:44[E]:LEU:HD23 | 1.86 | 0.40 |
| 10:ID:286:VAL:HG13 | 14:YF:100[D]:LYS:CE | 2.51 | 0.40 |
| 14:YF:209[B]:TYR:HB3 | 14:YF:324[B]:ILE:HG12 | 2.04 | 0.40 |
| 14:YF:290[E]:ASN:O | 14:YF:292[E]:TYR:N | 2.54 | 0.40 |
| 14:YF:345[C]:GLU:HB3 | 14:YF:352[C]:VAL:HG13 | 2.03 | 0.40 |
| 14:YF:367[E]:ILE:HG22 | 14:YF:367[E]:ILE:O | 2.21 | 0.40 |
| 14:YF:51[B]:MET:SD | 14:YF:108[B]:GLU:HA | 2.61 | 0.40 |
| 14:YF:10[D]:PRO:HB2 | 14:YF:74[D]:VAL:HG21 | 2.02 | 0.40 |
| 2:Z:750:VAL:HG23 | 2:Z:751:LEU:N | 2.37 | 0.40 |
| 15:ZA:26[C]:GLN:NE2 | 15:ZA:29[C]:VAL:H | 1.92 | 0.40 |
| 1:A:186:ILE:O | 1:A:187:ILE:HD13 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:657:PRO:O | 1:A:658:ILE:HD13 | 2.21 | 0.40 |
| 1:A:23:GLY:HA2 | 1:A:68:GLN:NE2 | 2.35 | 0.40 |
| 4:AA:147:THR:HB | 4:AA:163:SER:OG | 2.22 | 0.40 |
| 5:AD:130:PHE:CB | 5:AD:150:GLN:HB3 | 2.52 | 0.40 |
| 5:AD:136:VAL:HG21 | 5:AE:151:ILE:HD11 | 2.03 | 0.40 |
| 5:AE:357:SER:HB3 | 5:AE:358:VAL:H | 1.55 | 0.40 |
| 5:AE:390:LEU:HD23 | 5:AE:391:GLY:N | 2.36 | 0.40 |
| 6:AH:86:ASP:CG | 6:AH:180:GLN:HE21 | 2.19 | 0.40 |
| 7:AI:232:THR:HG23 | 7:AI:234:SER:N | 2.37 | 0.40 |
| 1:B:236:PHE:CD2 | 1:B:270:ILE:HD11 | 2.56 | 0.40 |
| 1:B:143:TYR:CE2 | 1:B:279:ASP:HB2 | 2.57 | 0.40 |
| 1:B:619:GLN:CD | 1:B:619:GLN:H | 2.21 | 0.40 |
| 7:BA:99:ARG:O | 7:BA:114:SER:HA | 2.21 | 0.40 |
| 8:BC:121:LYS:HG2 | 8:BC:122:THR:N | 2.37 | 0.40 |
| 9:BD:59:ASP:O | 9:BD:63:GLU:N | 2.55 | 0.40 |
| 11:BF:87:ILE:HD11 | 11:BF:167:ARG:CZ | 2.52 | 0.40 |
| 1:BH:251:ALA:HB2 | 1:BI:337:GLN:HG2 | 2.04 | 0.40 |
| 1:BI:515:PHE:O | 1:BI:537:ASP:HA | 2.21 | 0.40 |
| 2:BJ:160:VAL:CG1 | 2:BJ:592:GLY:HA2 | 2.52 | 0.40 |
| 2:BJ:472:LYS:HG3 | 2:BJ:474:GLU:HG3 | 2.03 | 0.40 |
| 2:BJ:548:ILE:O | 2:BJ:555:ARG:NH2 | 2.54 | 0.40 |
| 2:BJ:600:PHE:CE2 | 2:BJ:604:VAL:HB | 2.56 | 0.40 |
| 2:BJ:663:ASN:O | 2:BJ:667:PHE:N | 2.38 | 0.40 |
| 2:BJ:904:LEU:HD12 | 2:BJ:905:THR:N | 2.36 | 0.40 |
| 2:C:224:LEU:HD23 | 2:C:224:LEU:O | 2.20 | 0.40 |
| 2:C:411:LYS:O | 2:C:412:THR:HB | 2.21 | 0.40 |
| 2:C:627:GLU:HB2 | 2:C:628:HIS:CD2 | 2.56 | 0.40 |
| 2:C:643:PRO:HG2 | 11:V:84:TYR:CE2 | 2.56 | 0.40 |
| 2:C:78:TYR:O | 2:C:99:GLU:HB2 | 2.21 | 0.40 |
| 2:C:861:TYR:HE2 | 2:C:863:VAL:HG22 | 1.86 | 0.40 |
| 2:C:883:VAL:HG13 | 2:C:884:HIS:N | 2.36 | 0.40 |
| 2:C:986:ARG:HH12 | 3:D:323:ASP:HB2 | 1.87 | 0.40 |
| 3:CB:149:ASP:OD1 | 3:CB:150:LYS:N | 2.54 | 0.40 |
| 3:CA:13:THR:OG1 | 3:CB:310:ILE:HA | 2.21 | 0.40 |
| 4:CD:50:VAL:O | 4:CD:52:ASN:N | 2.54 | 0.40 |
| 5:CF:258:TYR:CE1 | 5:CF:384:THR:HG23 | 2.55 | 0.40 |
| 5:CF:84:GLY:C | 5:CF:86:VAL:H | 2.18 | 0.40 |
| 5:CF:590:GLN:OE1 | 5:CG:589:ILE:HA | 2.22 | 0.40 |
| 5:CG:469:PRO:HD3 | 5:CG:598:TRP:CE2 | 2.56 | 0.40 |
| 5:CG:11:VAL:HG22 | 5:CH:20:ARG:NE | 2.36 | 0.40 |
| 5:CH:321:ALA:O | 5:CH:324:VAL:HG12 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:CI:73:ASN:HB3 | 6:DA:69:THR:HA | 2.03 | 0.40 |
| 7:DB:227:VAL:HG23 | 7:DC:225:LYS:HB3 | 2.04 | 0.40 |
| 7:DB:295:ILE:HA | 7:DC:301:ARG:O | 2.21 | 0.40 |
| 7:DD:233:GLN:OE1 | 7:DD:252:GLY:HA3 | 2.21 | 0.40 |
| 8:DE:49:ILE:HG23 | 8:DE:60:VAL:O | 2.21 | 0.40 |
| 8:DF:49:ILE:HG23 | 8:DF:60:VAL:O | 2.21 | 0.40 |
| 2:BJ:662:SER:OG | 9:DG:14:GLU:O | 2.39 | 0.40 |
| 9:DG:58:SER:HB3 | 9:DG:61:LEU:HB3 | 2.03 | 0.40 |
| 3:E:175:ASP:OD1 | 3:E:176:ALA:N | 2.48 | 0.40 |
| 1:EA:108:THR:OG1 | 1:EA:109:GLU:N | 2.54 | 0.40 |
| 1:EA:186:ILE:O | 1:EA:187:ILE:HD13 | 2.21 | 0.40 |
| 1:EA:355:SER:O | 1:EA:379:LYS:HD3 | 2.21 | 0.40 |
| 1:EA:430:GLN:CD | 1:EA:430:GLN:H | 2.14 | 0.40 |
| 1:EB:347:THR:OG1 | 1:EB:348:PHE:N | 2.54 | 0.40 |
| 2:EC:307:ILE:HG22 | 2:EC:308:ALA:N | 2.36 | 0.40 |
| 2:EC:573:VAL:CG2 | 2:EC:610:ILE:HB | 2.51 | 0.40 |
| 2:EC:623:LEU:HD23 | 2:EC:623:LEU:HA | 1.82 | 0.40 |
| 1:EB:240:GLU:HB2 | 2:EC:719:LYS:HZ1 | 1.86 | 0.40 |
| 3:ED:147:LEU:HD21 | 3:ED:152:GLU:HB3 | 2.02 | 0.40 |
| 3:ED:38:PHE:HE1 | 3:ED:80:LYS:HG3 | 1.86 | 0.40 |
| 3:EE:147:LEU:CD2 | 3:EE:152:GLU:HG3 | 2.51 | 0.40 |
| 3:EE:204:THR:O | 3:EE:207:TYR:N | 2.49 | 0.40 |
| 4:EH:147:THR:HB | 4:EH:163:SER:OG | 2.22 | 0.40 |
| 4:EH:50:VAL:O | 4:EH:52:ASN:N | 2.54 | 0.40 |
| 5:EI:104:VAL:HG22 | 5:EI:105:ASN:H | 1.86 | 0.40 |
| 5:EI:289:LYS:HG3 | 5:EI:370:HIS:CE1 | 2.56 | 0.40 |
| 5:FA:192:ARG:CG | 5:FA:245:GLU:HB2 | 2.50 | 0.40 |
| 5:FA:497:PRO:HG2 | 5:FA:498:ASN:HD22 | 1.86 | 0.40 |
| 5:EJ:592:TYR:CG | 5:FA:499:PHE:HE1 | 2.38 | 0.40 |
| 5:FA:89:TYR:CE1 | 5:FA:137:TYR:CZ | 3.09 | 0.40 |
| 6:FC:109:VAL:HG13 | 6:FC:178:ILE:HG21 | 2.02 | 0.40 |
| 7:FE:85:LEU:O | 7:FE:88:PRO:HD2 | 2.21 | 0.40 |
| 7:FE:125:LEU:HD11 | 7:FF:125:LEU:HG | 2.03 | 0.40 |
| 7:FF:63:GLU:O | 7:FF:66:VAL:HG22 | 2.21 | 0.40 |
| 7:FG:289:GLN:N | 7:FG:289:GLN:OE1 | 2.55 | 0.40 |
| 8:FH:121:LYS:HG2 | 8:FH:122:THR:N | 2.36 | 0.40 |
| 8:FI:49:ILE:HG23 | 8:FI:60:VAL:O | 2.21 | 0.40 |
| 8:FI:69:TRP:HB2 | 8:FI:159:LEU:HD23 | 2.03 | 0.40 |
| 9:FJ:58:SER:HB3 | 9:FJ:61:LEU:HB3 | 2.03 | 0.40 |
| 11:GB:186:ARG:CG | 11:GB:187:ILE:H | 2.34 | 0.40 |
| 12:GC:225:ALA:HB1 | 12:GC:226:PRO:HD2 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:GD:413:TYR:HB2 | 1:GD:639:LEU:O | 2.21 | 0.40 |
| 1:GD:55:VAL:O | 1:GD:58:ASP:HB3 | 2.20 | 0.40 |
| 1:GE:342:ALA:C | 1:GE:344:ASP:N | 2.74 | 0.40 |
| 1:GE:424:TYR:CE2 | 1:GE:655:LEU:HD13 | 2.57 | 0.40 |
| 2:GF:411:LYS:O | 2:GF:412:THR:HB | 2.21 | 0.40 |
| 2:GF:447:ASN:OD1 | 2:GF:448:PHE:N | 2.54 | 0.40 |
| 2:GF:947:VAL:HA | 3:GG:118:PRO:CB | 2.45 | 0.40 |
| 3:GG:237:GLY:O | 3:GG:240:TYR:N | 2.48 | 0.40 |
| 3:GG:47:TRP:HH2 | 3:GG:58:PRO:HB3 | 1.82 | 0.40 |
| 3:GG:79:VAL:HG12 | 3:GG:80:LYS:O | 2.21 | 0.40 |
| 3:GH:147:LEU:CD2 | 3:GH:152:GLU:HG3 | 2.51 | 0.40 |
| 4:GI:35:PHE:CD1 | 4:GI:39:TYR:HE2 | 2.39 | 0.40 |
| 4:GJ:35:PHE:CD1 | 4:GJ:39:TYR:HE2 | 2.39 | 0.40 |
| 4:H:192:PHE:O | 4:H:261:VAL:N | 2.51 | 0.40 |
| 4:H:213:LYS:HE3 | 4:H:249:ILE:HG12 | 2.03 | 0.40 |
| 4:H:35:PHE:CD1 | 4:H:39:TYR:HE2 | 2.39 | 0.40 |
| 4:H:50:VAL:O | 4:H:52:ASN:N | 2.54 | 0.40 |
| 4:HA:213:LYS:HE3 | 4:HA:249:ILE:HG12 | 2.03 | 0.40 |
| 5:HB:163:ALA:HB3 | 5:HB:246:THR:HG22 | 2.04 | 0.40 |
| 5:HC:137:TYR:HB2 | 5:HC:143:TRP:HE1 | 1.86 | 0.40 |
| 5:HC:253:GLN:HB2 | 5:HC:255:ARG:NE | 2.37 | 0.40 |
| 5:HC:303:PRO:HD2 | 5:HC:365:ILE:HD13 | 2.02 | 0.40 |
| 5:HD:304:ILE:HG23 | 5:HD:385:TRP:CD1 | 2.56 | 0.40 |
| 5:HD:433:VAL:HG12 | 5:HD:434:GLU:N | 2.36 | 0.40 |
| 6:HE:11:ILE:O | 6:HG:7:LYS:HD2 | 2.21 | 0.40 |
| 6:HF:144:ASN:HA | 6:HF:161:LEU:HD23 | 2.03 | 0.40 |
| 6:HG:144:ASN:HA | 6:HG:161:LEU:HD23 | 2.04 | 0.40 |
| 7:HH:51:SER:HB3 | 7:HH:54:THR:HB | 2.03 | 0.40 |
| 7:HI:335:ASN:OD1 | 7:HI:336:GLU:N | 2.53 | 0.40 |
| 7:HI:515:TRP:CZ3 | 7:HJ:439:ILE:HG12 | 2.56 | 0.40 |
| 5:I:137:TYR:HA | 5:I:143:TRP:CD1 | 2.55 | 0.40 |
| 5:I:89:TYR:CZ | 5:I:139:ALA:HA | 2.56 | 0.40 |
| 5:I:163:ALA:HB3 | 5:I:246:THR:HG22 | 2.04 | 0.40 |
| 8:IB:10:PHE:CD2 | 8:IB:15:PHE:CE1 | 3.10 | 0.40 |
| 9:IC:85:GLU:OE2 | 9:IC:87:ARG:NH2 | 2.53 | 0.40 |
| 10:ID:311:PHE:HB3 | 10:ID:312:GLY:H | 1.44 | 0.40 |
| 11:IE:50:ILE:HD11 | 11:IE:169:ILE:CD1 | 2.51 | 0.40 |
| 5:J:592:TYR:CG | 5:K:499:PHE:HE1 | 2.39 | 0.40 |
| 5:K:120:SER:OG | 5:K:122:VAL:HG22 | 2.21 | 0.40 |
| 5:K:394:LEU:HD23 | 5:K:394:LEU:HA | 1.91 | 0.40 |
| 5:J:443:PHE:O | 5:K:408:VAL:HG13 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:544:VAL:HA | 5:K:569:TYR:CE1 | 2.56 | 0.40 |
| 5:J:340:VAL:HG22 | 6:N:173:THR:HA | 2.04 | 0.40 |
| 6:N:200:THR:HA | 6:N:211:VAL:HA | 2.03 | 0.40 |
| 6:N:26:ASP:HB3 | 6:N:34:SER:HA | 2.03 | 0.40 |
| 7:O:44:VAL:HB | 7:P:24:ASN:ND2 | 2.35 | 0.40 |
| 7:O:520:ASN:ND2 | 7:P:434:VAL:HG21 | 2.36 | 0.40 |
| 8:S:89:GLN:HB3 | 8:S:134:PRO:CG | 2.50 | 0.40 |
| 1:B:69:GLN:NE2 | 11:V:74:LEU:HD23 | 2.36 | 0.40 |
| 1:X:108:THR:OG1 | 1:X:109:GLU:N | 2.54 | 0.40 |
| 1:X:401:LEU:HD12 | 1:X:401:LEU:H | 1.86 | 0.40 |
| 1:X:433:GLU:OE2 | 1:X:655:LEU:HD11 | 2.20 | 0.40 |
| 1:Y:190:LYS:O | 1:Y:191:ASN:HB2 | 2.20 | 0.40 |
| 1:X:251:ALA:CB | 1:Y:337:GLN:HG2 | 2.51 | 0.40 |
| 13:YA:209[E]:GLN:HB3 | 13:YA:211[E]:VAL:HG23 | 2.03 | 0.40 |
| 13:YA:227[E]:ARG:HG2 | 13:YA:228[E]:GLU:N | 2.36 | 0.40 |
| 13:YA:266[F]:TRP:NE1 | 13:YA:274[F]:GLN:HG2 | 2.36 | 0.40 |
| 13:YA:47[C]:ILE:HG23 | 14:YD:123[C]:PRO:CG | 2.49 | 0.40 |
| 13:YB:266[F]:TRP:NE1 | 13:YB:274[F]:GLN:HG2 | 2.36 | 0.40 |
| 13:YB:34[E]:LEU:HD13 | 14:YE:163[E]:THR:CG2 | 2.47 | 0.40 |
| 13:YB:373[C]:ARG:HA | 13:YB:373[C]:ARG:NE | 2.30 | 0.40 |
| 13:YA:463[C]:ILE:O | 13:YB:455[C]:LYS:HA | 2.21 | 0.40 |
| 13:YB:490[D]:VAL:HG21 | 13:YC:486[D]:GLU:HB2 | 2.02 | 0.40 |
| 13:YB:76[A]:PRO:HG3 | 13:YB:96[A]:VAL:CB | 2.50 | 0.40 |
| 13:YC:187[E]:ARG:HD3 | 13:YC:187[E]:ARG:HA | 1.86 | 0.40 |
| 13:YB:432[C]:ARG:NH1 | 13:YC:432[C]:ARG:HD2 | 2.36 | 0.40 |
| 13:YB:444[F]:ALA:HB3 | 13:YC:437[F]:ASN:N | 2.36 | 0.40 |
| 13:YB:506[A]:VAL:HA | 13:YC:498[A]:VAL:O | 2.21 | 0.40 |
| 13:YC:534[F]:LEU:HD11 | 13:YC:536[F]:TRP:NE1 | 2.32 | 0.40 |
| 13:YA:561[F]:SER:O | 13:YC:569[F]:GLY:HA2 | 2.21 | 0.40 |
| 13:YC:81[B]:ARG:HD3 | 14:YE:261[B]:SER:HA | 2.02 | 0.40 |
| 14:YD:51[E]:MET:SD | 14:YD:108[E]:GLU:HA | 2.61 | 0.40 |
| 14:YD:10[C]:PRO:HB2 | 14:YD:74[C]:VAL:HG21 | 2.03 | 0.40 |
| 14:YD:136[D]:LEU:HD21 | 14:YD:166[D]:PHE:CE2 | 2.56 | 0.40 |
| 14:YD:330[C]:LYS:HG2 | 14:YE:101[C]:GLY:HA3 | 2.03 | 0.40 |
| 14:YD:367[C]:ILE:HG22 | 14:YD:367[C]:ILE:O | 2.21 | 0.40 |
| 14:YD:367[E]:ILE:HG22 | 14:YD:367[E]:ILE:O | 2.21 | 0.40 |
| 14:YD:373[C]:LYS:HB3 | 14:YD:373[C]:LYS:HE2 | 1.87 | 0.40 |
| 14:YE:136[B]:LEU:HD21 | 14:YE:166[B]:PHE:CE2 | 2.56 | 0.40 |
| 14:YE:210[D]:PRO:HB2 | 14:YE:228[D]:TYR:CD2 | 2.56 | 0.40 |
| 14:YE:212[F]:ILE:HG12 | 14:YE:228[F]:TYR:HB2 | 2.02 | 0.40 |
| 14:YE:290[A]:ASN:O | 14:YE:292[A]:TYR:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:YE:290[D]:ASN:O | 14:YE:292[D]:TYR:N | 2.54 | 0.40 |
| 14:YE:16[B]:LEU:CD2 | 14:YE:29[B]:VAL:HB | 2.52 | 0.40 |
| 14:YE:16[C]:LEU:CD2 | 14:YE:29[C]:VAL:HB | 2.52 | 0.40 |
| 14:YF:136[B]:LEU:HD23 | 14:YF:136[B]:LEU:HA | 1.84 | 0.40 |
| 14:YF:136[A]:LEU:HD21 | 14:YF:166[A]:PHE:CE2 | 2.56 | 0.40 |
| 14:YF:174[A]:ARG:HG3 | 14:YF:188[A]:VAL:HG22 | 2.03 | 0.40 |
| 14:YF:210[C]:PRO:HB2 | 14:YF:228[C]:TYR:CD2 | 2.56 | 0.40 |
| 14:YF:212[B]:ILE:HG12 | 14:YF:228[B]:TYR:HB2 | 2.03 | 0.40 |
| 13:YA:100[E]:TYR:CD2 | 14:YF:258[E]:PHE:HD1 | 2.39 | 0.40 |
| 14:YF:279[E]:ARG:HA | 14:YF:279[E]:ARG:HD3 | 1.43 | 0.40 |
| 14:YF:307[C]:TYR:HD1 | 14:YF:307[C]:TYR:HA | 1.66 | 0.40 |
| 14:YF:47[F]:ARG:NH1 | 14:YF:341[F]:GLU:OE1 | 2.54 | 0.40 |
| 14:YF:38[B]:LEU:HB3 | 14:YF:346[B]:LEU:HG | 2.03 | 0.40 |
| 14:YF:367[A]:ILE:HG22 | 14:YF:367[A]:ILE:O | 2.21 | 0.40 |
| 2:Z:362:LYS:O | 2:Z:382:GLU:HG3 | 2.21 | 0.40 |
| 2:Z:196:GLU:HB3 | 2:Z:520:SER:OG | 2.21 | 0.40 |
| 2:Z:573:VAL:CG2 | 2:Z:610:ILE:HB | 2.51 | 0.40 |
| 2:Z:683:TYR:O | 2:Z:686:LEU:N | 2.53 | 0.40 |
| 2:Z:852:ILE:HG21 | 2:Z:854:TYR:CZ | 2.56 | 0.40 |
| 15:ZA:56[E]:HIS:CD2 | 15:ZA:83[E]:CYS:HB2 | 2.57 | 0.40 |
| 1:A:429:LEU:HD12 | 1:A:429:LEU:O | 2.21 | 0.40 |
| 1:A:507:ASP:HA | 1:A:597:TYR:CZ | 2.56 | 0.40 |
| 4:AA:145:LYS:O | 4:AA:164:ILE:HA | 2.22 | 0.40 |
| 4:AA:205:THR:HG22 | 4:AB:284:ILE:HD11 | 2.02 | 0.40 |
| 4:AA:213:LYS:HE3 | 4:AA:249:ILE:HG12 | 2.03 | 0.40 |
| 4:AA:54:THR:HA | 4:AB:7:LYS:O | 2.21 | 0.40 |
| 5:AD:258:TYR:HA | 5:AD:385:TRP:O | 2.21 | 0.40 |
| 5:AD:89:TYR:HA | 5:AD:137:TYR:CD2 | 2.57 | 0.40 |
| 5:AE:153:LYS:HG3 | 5:AE:153:LYS:O | 2.21 | 0.40 |
| 5:AE:285:LEU:CD2 | 5:AE:375:PHE:H | 2.35 | 0.40 |
| 5:AE:377:HIS:CG | 5:AE:378:GLY:H | 2.40 | 0.40 |
| 6:AF:109:VAL:HG13 | 6:AF:178:ILE:HG21 | 2.02 | 0.40 |
| 6:AG:109:VAL:HG13 | 6:AG:178:ILE:HG21 | 2.02 | 0.40 |
| 7:AI:443:SER:HA | 7:BA:509:GLY:O | 2.21 | 0.40 |
| 7:AI:520:ASN:ND2 | 7:AJ:434:VAL:HG21 | 2.36 | 0.40 |
| 1:B:344:ASP:O | 1:B:347:THR:OG1 | 2.37 | 0.40 |
| 1:B:485:VAL:HG22 | 1:B:624:TYR:CD1 | 2.55 | 0.40 |
| 1:B:62:TYR:CZ | 1:B:66:TYR:HE2 | 2.38 | 0.40 |
| 8:BB:69:TRP:HB2 | 8:BB:159:LEU:HD23 | 2.03 | 0.40 |
| 8:BC:24:GLU:N | 8:BC:112:ILE:O | 2.48 | 0.40 |
| 8:BC:69:TRP:HB2 | 8:BC:159:LEU:HD23 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:BD:62:PHE:HZ | 9:BD:127:ALA:HA | 1.86 | 0.40 |
| 11:BF:43:TYR:CE2 | 11:BF:180:PHE:HB2 | 2.49 | 0.40 |
| 12:BG:23:SER:O | 12:BG:202:ASN:N | 2.46 | 0.40 |
| 1:BH:186:ILE:O | 1:BH:187:ILE:HD13 | 2.22 | 0.40 |
| 1:BH:429:LEU:HD12 | 1:BH:429:LEU:O | 2.21 | 0.40 |
| 1:BI:401:LEU:HD23 | 1:BI:401:LEU:HA | 1.87 | 0.40 |
| 1:BI:58:ASP:O | 1:BI:59:LEU:C | 2.60 | 0.40 |
| 2:BJ:306:ARG:C | 2:BJ:307:ILE:HD12 | 2.41 | 0.40 |
| 2:BJ:340:PRO:C | 2:BJ:342:SER:H | 2.25 | 0.40 |
| 2:BJ:514:PHE:HD1 | 2:BJ:525:TRP:HB2 | 1.85 | 0.40 |
| 2:BJ:852:ILE:HG21 | 2:BJ:854:TYR:CZ | 2.56 | 0.40 |
| 2:C:217:GLN:HG2 | 2:C:218:THR:N | 2.36 | 0.40 |
| 2:C:412:THR:OG1 | 2:C:413:TRP:N | 2.53 | 0.40 |
| 2:C:548:ILE:O | 2:C:555:ARG:NH2 | 2.54 | 0.40 |
| 3:CB:47:TRP:NE1 | 3:CB:270:ARG:HD2 | 2.37 | 0.40 |
| 4:CC:50:VAL:O | 4:CC:52:ASN:N | 2.54 | 0.40 |
| 4:CE:35:PHE:CD1 | 4:CE:39:TYR:HE2 | 2.39 | 0.40 |
| 4:CE:50:VAL:O | 4:CE:52:ASN:N | 2.54 | 0.40 |
| 5:CF:151:ILE:O | 5:CF:152:ASP:HB3 | 2.21 | 0.40 |
| 5:CF:425:PHE:HD2 | 7:HJ:495:GLN:HA | 1.86 | 0.40 |
| 5:CF:461:GLU:OE2 | 5:CF:597:ARG:NE | 2.46 | 0.40 |
| 5:CF:572:ALA:HA | 5:CG:540:GLU:HG2 | 2.02 | 0.40 |
| 5:CG:136:VAL:HG21 | 5:CH:151:ILE:HD11 | 2.03 | 0.40 |
| 5:CG:492:GLU:O | 5:CG:514:HIS:HE1 | 2.04 | 0.40 |
| 5:CG:559:PRO:HA | 5:CG:561:GLU:OE2 | 2.20 | 0.40 |
| 5:CG:568:LYS:HG2 | 5:CH:551:ILE:HG13 | 2.03 | 0.40 |
| 5:CH:177:PHE:O | 5:CH:230:ILE:HG13 | 2.21 | 0.40 |
| 5:CF:264:ARG:HD3 | 5:CH:327:PRO:HG3 | 2.04 | 0.40 |
| 5:CH:303:PRO:HD2 | 5:CH:365:ILE:HD13 | 2.02 | 0.40 |
| 5:CG:569:TYR:CE1 | 5:CH:544:VAL:HG22 | 2.55 | 0.40 |
| 6:CJ:79:PRO:HD2 | 6:CJ:193:TRP:CB | 2.51 | 0.40 |
| 3:D:147:LEU:HD21 | 3:D:152:GLU:HB3 | 2.02 | 0.40 |
| 6:DA:126:VAL:HG13 | 6:DA:156:LEU:HD11 | 2.03 | 0.40 |
| 7:DB:474:GLY:O | 7:DC:472:ARG:HG2 | 2.21 | 0.40 |
| 7:DC:146:SER:HA | 7:DC:164:LYS:HZ3 | 1.82 | 0.40 |
| 7:DC:453:GLU:HG3 | 7:DC:475:LEU:HD11 | 2.03 | 0.40 |
| 7:DD:232:THR:HG23 | 7:DD:235:GLU:H | 1.85 | 0.40 |
| 7:DD:32:VAL:O | 7:DD:36:ILE:HG12 | 2.21 | 0.40 |
| 8:DE:10:PHE:CE1 | 8:FH:35:GLN:HG2 | 2.56 | 0.40 |
| 11:DI:160:VAL:O | 11:DI:164:GLU:N | 2.54 | 0.40 |
| 12:DJ:215:MET:CE | 12:GC:99:SER:HB2 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:EA:132:LEU:HD23 | 1:EA:132:LEU:HA | 1.77 | 0.40 |
| 1:EA:227:ARG:HH21 | 1:EB:81:ARG:HH21 | 1.69 | 0.40 |
| 1:EA:251:ALA:CB | 1:EB:337:GLN:HG2 | 2.51 | 0.40 |
| 1:EB:352:ARG:O | 1:EB:353:PHE:HB2 | 2.21 | 0.40 |
| 1:EB:464:MET:HG3 | 1:EB:465:LEU:N | 2.36 | 0.40 |
| 1:EB:46:TYR:HB3 | 1:EB:53:LEU:HD23 | 2.02 | 0.40 |
| 1:EA:227:ARG:NH2 | 1:EB:81:ARG:HH21 | 2.19 | 0.40 |
| 2:EC:160:VAL:CG1 | 2:EC:592:GLY:HA2 | 2.52 | 0.40 |
| 2:EC:796:THR:HG23 | 2:EC:797:TYR:HD2 | 1.86 | 0.40 |
| 3:ED:13:THR:OG1 | 3:EE:310:ILE:HA | 2.21 | 0.40 |
| 3:EE:28:ILE:HG22 | 3:EE:83:PRO:HG3 | 2.04 | 0.40 |
| 4:EF:168:PHE:CZ | 4:EG:149:ARG:HB3 | 2.57 | 0.40 |
| 4:EG:65:GLY:HA3 | 4:EG:84:ARG:NH1 | 2.36 | 0.40 |
| 5:EI:154:ILE:HG23 | 5:EJ:153:LYS:HZ1 | 1.85 | 0.40 |
| 5:EI:304:ILE:HD11 | 5:EI:308:SER:O | 2.22 | 0.40 |
| 5:EI:490:TRP:NE1 | 5:EI:500:ALA:O | 2.55 | 0.40 |
| 5:EI:7:ILE:HG22 | 5:EI:8:GLY:O | 2.22 | 0.40 |
| 5:EJ:130:PHE:CB | 5:EJ:150:GLN:HB3 | 2.52 | 0.40 |
| 5:EJ:144:GLU:N | 5:EJ:144:GLU:OE1 | 2.54 | 0.40 |
| 5:EJ:253:GLN:HB2 | 5:EJ:255:ARG:NE | 2.37 | 0.40 |
| 5:EJ:262:GLN:HA | 5:EJ:381:ILE:O | 2.20 | 0.40 |
| 5:EJ:289:LYS:HG3 | 5:EJ:370:HIS:CE1 | 2.57 | 0.40 |
| 5:EJ:496:ASP:OD2 | 5:EJ:499:PHE:HB2 | 2.22 | 0.40 |
| 5:EJ:469:PRO:HD3 | 5:EJ:598:TRP:CE2 | 2.56 | 0.40 |
| 4:F:145:LYS:O | 4:F:164:ILE:HA | 2.22 | 0.40 |
| 5:EI:407:TYR:CD1 | 5:FA:407:TYR:HB2 | 2.56 | 0.40 |
| 5:FA:67:SER:CB | 5:FA:94:ARG:HB2 | 2.51 | 0.40 |
| 5:FA:340:VAL:HG22 | 6:FB:172:SER:O | 2.22 | 0.40 |
| 6:FC:70:ILE:HG13 | 6:FD:212:PHE:CD1 | 2.56 | 0.40 |
| 5:EI:318:GLN:NE2 | 6:FD:4:LEU:O | 2.52 | 0.40 |
| 7:FE:98:THR:O | 7:FF:95:TYR:HA | 2.21 | 0.40 |
| 8:FH:89:GLN:HB3 | 8:FH:134:PRO:CG | 2.50 | 0.40 |
| 8:FI:121:LYS:HG2 | 8:FI:122:THR:N | 2.37 | 0.40 |
| 12:GC:185:VAL:HG23 | 12:GC:186:THR:N | 2.35 | 0.40 |
| 1:GD:186:ILE:O | 1:GD:187:ILE:HD13 | 2.21 | 0.40 |
| 1:GD:201:VAL:HG21 | 1:GD:262:PRO:HB3 | 2.02 | 0.40 |
| 1:GE:494:THR:HG22 | 1:GE:498:GLY:HA2 | 2.03 | 0.40 |
| 1:GE:565:GLU:OE1 | 1:GE:571:PRO:HD3 | 2.20 | 0.40 |
| 3:E:228:ASN:HB2 | 2:GF:483:LYS:HZ3 | 1.87 | 0.40 |
| 2:GF:577:GLY:N | 2:GF:606:ASP:O | 2.54 | 0.40 |
| 4:GJ:147:THR:HB | 4:GJ:163:SER:OG | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:HD:342:CYS:HB3 | 5:HD:349:TRP:CH2 | 2.57 | 0.40 |
| 5:HD:357:SER:N | 5:HD:372:ASP:OD1 | 2.54 | 0.40 |
| 6:HF:145:SER:O | 6:HF:159:THR:N | 2.45 | 0.40 |
| 7:HH:424:ARG:O | 7:HI:504:ARG:NH2 | 2.50 | 0.40 |
| 7:HI:422:LYS:HB3 | 7:HJ:504:ARG:HA | 2.04 | 0.40 |
| 7:HJ:196:VAL:CG2 | 7:HJ:214:THR:HG22 | 2.52 | 0.40 |
| 7:HJ:475:LEU:HD23 | 7:HJ:475:LEU:HA | 1.83 | 0.40 |
| 5:I:162:VAL:HA | 5:I:246:THR:O | 2.20 | 0.40 |
| 5:I:477:SER:O | 5:I:601:ILE:N | 2.50 | 0.40 |
| 11:IE:87:ILE:HD11 | 11:IE:167:ARG:CZ | 2.51 | 0.40 |
| 5:J:98:VAL:HG12 | 5:J:99:PHE:CD2 | 2.46 | 0.40 |
| 5:K:97:ASP:OD1 | 5:K:102:TRP:CE2 | 2.74 | 0.40 |
| 5:K:304:ILE:HG23 | 5:K:385:TRP:CD1 | 2.56 | 0.40 |
| 5:K:565:ILE:O | 5:K:565:ILE:HG13 | 2.21 | 0.40 |
| 6:L:70:ILE:HD12 | 6:L:196:LEU:HD11 | 2.03 | 0.40 |
| 6:M:109:VAL:HG13 | 6:M:178:ILE:HG21 | 2.02 | 0.40 |
| 6:N:42:GLN:N | 6:N:42:GLN:OE1 | 2.52 | 0.40 |
| 7:O:232:THR:HG23 | 7:O:234:SER:N | 2.37 | 0.40 |
| 5:I:196:ARG:CD | 7:O:5:THR:HG23 | 2.52 | 0.40 |
| 7:Q:196:VAL:CG2 | 7:Q:214:THR:HG22 | 2.52 | 0.40 |
| 8:R:69:TRP:HB2 | 8:R:159:LEU:HD23 | 2.03 | 0.40 |
| 9:T:62:PHE:HZ | 9:T:127:ALA:HA | 1.86 | 0.40 |
| 10:U:62:LEU:HD12 | 10:U:62:LEU:HA | 1.88 | 0.40 |
| 11:V:87:ILE:HD11 | 11:V:167:ARG:CZ | 2.51 | 0.40 |
| 1:X:110:ILE:HA | 1:X:110:ILE:HD12 | 1.90 | 0.40 |
| 1:X:111:MET:HA | 1:X:164:ARG:HA | 2.03 | 0.40 |
| 1:X:201:VAL:HG21 | 1:X:262:PRO:HB3 | 2.02 | 0.40 |
| 1:Y:448:TYR:HD1 | 1:Y:452:VAL:HG11 | 1.85 | 0.40 |
| 1:Y:496:GLU:H | 1:Y:496:GLU:HG2 | 1.57 | 0.40 |
| 13:YA:16[B]:GLU:OE2 | 13:YA:49[B]:THR:OG1 | 2.40 | 0.40 |
| 13:YA:266[D]:TRP:NE1 | 13:YA:274[D]:GLN:HG2 | 2.36 | 0.40 |
| 13:YA:277[D]:LEU:HD23 | 13:YA:277[D]:LEU:HA | 1.80 | 0.40 |
| 13:YA:318[F]:GLN:NE2 | 13:YB:367[F]:PRO:HB2 | 2.37 | 0.40 |
| 13:YA:396[B]:GLU:HA | 13:YC:69[B]:ILE:CD1 | 2.51 | 0.40 |
| 13:YA:393[F]:MET:O | 13:YA:400[F]:ILE:HA | 2.21 | 0.40 |
| 13:YA:148[D]:GLN:HG3 | 13:YA:421[D]:TYR:CE1 | 2.56 | 0.40 |
| 13:YA:76[A]:PRO:HB2 | 13:YA:98[A]:GLY:CA | 2.51 | 0.40 |
| 13:YB:16[F]:GLU:OE2 | 13:YB:49[F]:THR:OG1 | 2.39 | 0.40 |
| 13:YB:180[A]:LEU:HD13 | 13:YB:180[A]:LEU:HA | 1.76 | 0.40 |
| 13:YB:266[B]:TRP:NE1 | 13:YB:274[B]:GLN:HG2 | 2.36 | 0.40 |
| 13:YB:399[F]:HIS:ND1 | 13:YB:417[F]:PRO:HD3 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YB:471[D]:LEU:O | 13:YC:463[D]:ILE:HA | 2.22 | 0.40 |
| 13:YB:552[C]:GLU:HB2 | 13:YB:554[C]:MET:HE1 | 2.03 | 0.40 |
| 13:YB:92[E]:THR:HB | 14:YE:282[E]:ALA:HB2 | 2.04 | 0.40 |
| 13:YC:209[A]:GLN:HB3 | 13:YC:211[A]:VAL:HG23 | 2.02 | 0.40 |
| 13:YC:209[F]:GLN:HE21 | 13:YC:209[F]:GLN:HB2 | 1.65 | 0.40 |
| 13:YC:227[A]:ARG:HG2 | 13:YC:228[A]:GLU:N | 2.36 | 0.40 |
| 13:YC:399[E]:HIS:ND1 | 13:YC:417[E]:PRO:HD3 | 2.36 | 0.40 |
| 13:YC:393[C]:MET:O | 13:YC:400[C]:ILE:HA | 2.22 | 0.40 |
| 13:YB:450[A]:VAL:HG11 | 13:YC:446[A]:GLY:H | 1.85 | 0.40 |
| 13:YB:490[A]:VAL:HG21 | 13:YC:486[A]:GLU:HB2 | 2.02 | 0.40 |
| 13:YC:76[D]:PRO:HG3 | 13:YC:96[D]:VAL:CB | 2.50 | 0.40 |
| 13:YC:90[C]:TRP:O | 13:YC:92[C]:THR:HG23 | 2.21 | 0.40 |
| 14:YD:51[F]:MET:SD | 14:YD:108[F]:GLU:HA | 2.61 | 0.40 |
| 14:YD:136[F]:LEU:HD23 | 14:YD:136[F]:LEU:HA | 1.84 | 0.40 |
| 14:YD:15[E]:LYS:HE2 | 14:YD:15[E]:LYS:HB3 | 1.54 | 0.40 |
| 14:YD:212[B]:ILE:HG12 | 14:YD:228[B]:TYR:HB2 | 2.03 | 0.40 |
| 11:V:190:LYS:NZ | 14:YD:24[B]:SER:HA | 2.35 | 0.40 |
| 14:YD:16[E]:LEU:CD2 | 14:YD:29[E]:VAL:HB | 2.52 | 0.40 |
| 14:YD:209[C]:TYR:HB3 | 14:YD:324[C]:ILE:HG12 | 2.04 | 0.40 |
| 14:YD:47[C]:ARG:NH1 | 14:YD:341[C]:GLU:OE1 | 2.54 | 0.40 |
| 14:YD:75[D]:ALA:HB2 | 14:YD:83[D]:VAL:HA | 2.01 | 0.40 |
| 14:YE:307[E]:TYR:HA | 14:YE:307[E]:TYR:HD1 | 1.66 | 0.40 |
| 14:YE:66[D]:GLY:O | 14:YE:90[D]:CYS:HB3 | 2.21 | 0.40 |
| 14:YF:145[E]:LEU:HG | 14:YF:145[E]:LEU:H | 1.70 | 0.40 |
| 14:YF:136[F]:LEU:HD21 | 14:YF:166[F]:PHE:CE2 | 2.56 | 0.40 |
| 14:YF:16[E]:LEU:HD22 | 14:YF:31[E]:LEU:HD21 | 2.03 | 0.40 |
| 14:YF:170[F]:LEU:HD23 | 14:YF:170[F]:LEU:HA | 1.69 | 0.40 |
| 14:YF:212[F]:ILE:HG12 | 14:YF:228[F]:TYR:HB2 | 2.02 | 0.40 |
| 14:YF:290[B]:ASN:O | 14:YF:292[B]:TYR:N | 2.54 | 0.40 |
| 14:YF:16[B]:LEU:CD2 | 14:YF:29[B]:VAL:HB | 2.52 | 0.40 |
| 14:YF:10[C]:PRO:HB2 | 14:YF:74[C]:VAL:HG21 | 2.03 | 0.40 |
| 2:Z:251:ASP:OD2 | 2:Z:252:LYS:HG3 | 2.20 | 0.40 |
| 1:A:355:SER:O | 1:A:379:LYS:HD3 | 2.21 | 0.40 |
| 1:A:501:TYR:O | 1:A:503:ASN:ND2 | 2.50 | 0.40 |
| 4:AA:192:PHE:O | 4:AA:261:VAL:N | 2.51 | 0.40 |
| 5:AC:275:SER:OG | 5:AC:282:VAL:N | 2.52 | 0.40 |
| 5:AC:304:ILE:HD12 | 5:AC:384:THR:O | 2.21 | 0.40 |
| 5:AC:490:TRP:NE1 | 5:AC:500:ALA:O | 2.55 | 0.40 |
| 5:AD:323:THR:HG21 | 5:AD:354:THR:HG23 | 2.02 | 0.40 |
| 5:AD:326:MET:CE | 5:AE:264:ARG:HB3 | 2.51 | 0.40 |
| 5:AC:89:TYR:HB3 | 5:AD:98:VAL:HG13 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AE:30:PHE:O | 5:AE:31:ASP:C | 2.60 | 0.40 |
| 5:AE:506:LEU:HD22 | 5:AE:510:GLY:O | 2.22 | 0.40 |
| 6:AG:144:ASN:HA | 6:AG:161:LEU:HD23 | 2.04 | 0.40 |
| 7:AI:85:LEU:O | 7:AI:88:PRO:HD2 | 2.21 | 0.40 |
| 1:B:394:ASN:O | 1:B:397:LYS:HG2 | 2.21 | 0.40 |
| 1:B:424:TYR:CE2 | 1:B:655:LEU:HD13 | 2.57 | 0.40 |
| 7:AJ:229:LYS:HD3 | 7:BA:222:GLU:O | 2.22 | 0.40 |
| 8:BB:49:ILE:HG23 | 8:BB:60:VAL:O | 2.21 | 0.40 |
| 11:BF:146:TYR:HE2 | 11:BF:150:LEU:HD23 | 1.85 | 0.40 |
| 12:BG:30:PRO:HG2 | 12:BG:177:TRP:HE1 | 1.86 | 0.40 |
| 1:BH:302:GLU:HG2 | 1:BH:303:ASN:N | 2.36 | 0.40 |
| 1:BH:418:THR:HG22 | 1:BH:482:ILE:HG22 | 2.02 | 0.40 |
| 1:BH:414:LEU:HD21 | 1:BH:486:ARG:HH21 | 1.85 | 0.40 |
| 1:BI:226:MET:SD | 1:BI:236:PHE:CE1 | 3.15 | 0.40 |
| 1:BI:240:GLU:O | 1:BI:240:GLU:HG2 | 2.21 | 0.40 |
| 1:BH:251:ALA:CB | 1:BI:337:GLN:HG2 | 2.51 | 0.40 |
| 1:BI:342:ALA:C | 1:BI:344:ASP:N | 2.74 | 0.40 |
| 1:BI:368:LYS:O | 1:BI:368:LYS:HG3 | 2.22 | 0.40 |
| 1:BI:59:LEU:HD22 | 2:BJ:668:CYS:SG | 2.60 | 0.40 |
| 2:BJ:821:ILE:N | 2:BJ:824:GLN:NE2 | 2.69 | 0.40 |
| 2:C:152:GLN:OE1 | 2:C:152:GLN:N | 2.31 | 0.40 |
| 2:C:186:ASP:HB3 | 2:C:189:ARG:HG3 | 2.03 | 0.40 |
| 2:C:223:LYS:C | 2:C:225:PHE:H | 2.25 | 0.40 |
| 2:C:376:PHE:HB2 | 2:C:405:VAL:HA | 2.02 | 0.40 |
| 2:C:577:GLY:N | 2:C:606:ASP:O | 2.54 | 0.40 |
| 2:C:750:VAL:HG23 | 2:C:751:LEU:N | 2.37 | 0.40 |
| 3:CB:131:TYR:CD1 | 3:CB:190:TYR:HA | 2.57 | 0.40 |
| 3:CB:138:ASP:HA | 3:CB:150:LYS:CE | 2.52 | 0.40 |
| 3:CB:272:ILE:HB | 3:CB:313:GLU:HB3 | 2.03 | 0.40 |
| 3:CB:268:GLY:HA3 | 3:CB:318:ILE:O | 2.20 | 0.40 |
| 4:CD:65:GLY:HA3 | 4:CD:84:ARG:NH1 | 2.36 | 0.40 |
| 4:CE:147:THR:HB | 4:CE:163:SER:OG | 2.22 | 0.40 |
| 4:CD:216:THR:HG23 | 4:CE:222:LEU:HD13 | 2.03 | 0.40 |
| 5:CF:89:TYR:CZ | 5:CF:139:ALA:HA | 2.56 | 0.40 |
| 2:BJ:1001:PHE:CE2 | 5:CF:5:ILE:HD11 | 2.56 | 0.40 |
| 5:CG:85:THR:OG1 | 5:CG:137:TYR:CZ | 2.73 | 0.40 |
| 5:CG:186:TYR:HB3 | 5:CG:227:GLY:O | 2.20 | 0.40 |
| 5:CG:181:PHE:HE2 | 5:CG:246:THR:HG22 | 1.87 | 0.40 |
| 6:CI:79:PRO:HD2 | 6:CI:193:TRP:CB | 2.51 | 0.40 |
| 6:CI:26:ASP:HB3 | 6:CI:34:SER:HA | 2.03 | 0.40 |
| 6:CJ:144:ASN:HA | 6:CJ:161:LEU:HD23 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:13:THR:OG1 | 3:E:310:ILE:HA | 2.22 | 0.40 |
| 6:DA:71:ILE:O | 6:DA:215:PHE:N | 2.36 | 0.40 |
| 7:DB:315:ILE:O | 7:DC:321:MET:HA | 2.22 | 0.40 |
| 7:DB:85:LEU:O | 7:DB:88:PRO:HD2 | 2.21 | 0.40 |
| 7:DC:223:GLU:HG3 | 7:DC:224:TYR:CE1 | 2.57 | 0.40 |
| 7:DD:375:TYR:OH | 7:DD:392:LEU:HD23 | 2.21 | 0.40 |
| 9:DG:68:LEU:HA | 9:DG:68:LEU:HD23 | 1.88 | 0.40 |
| 10:DH:285:LEU:HA | 14:YF:215[F]:GLU:HG2 | 2.03 | 0.40 |
| 11:DI:43:TYR:CE2 | 11:DI:180:PHE:HB2 | 2.49 | 0.40 |
| 11:DI:50:ILE:HD11 | 11:DI:169:ILE:HD11 | 2.03 | 0.40 |
| 11:DI:2:LEU:CD1 | 11:DI:71:TRP:CE2 | 3.02 | 0.40 |
| 11:DI:74:LEU:HD11 | 11:DI:79:ASN:ND2 | 2.37 | 0.40 |
| 3:E:235:ASP:O | 3:E:236:PHE:HB2 | 2.20 | 0.40 |
| 1:EA:251:ALA:HB2 | 1:EB:337:GLN:HG2 | 2.03 | 0.40 |
| 1:EB:125:ILE:O | 1:EB:150:ASP:HA | 2.22 | 0.40 |
| 1:EB:236:PHE:CD2 | 1:EB:270:ILE:HD11 | 2.57 | 0.40 |
| 1:EB:342:ALA:C | 1:EB:344:ASP:N | 2.74 | 0.40 |
| 1:EB:537:ASP:N | 1:EB:537:ASP:OD1 | 2.46 | 0.40 |
| 2:EC:548:ILE:O | 2:EC:555:ARG:NH2 | 2.54 | 0.40 |
| 2:EC:821:ILE:N | 2:EC:824:GLN:NE2 | 2.69 | 0.40 |
| 2:EC:975:ASN:HA | 2:EC:981:GLN:CB | 2.52 | 0.40 |
| 3:ED:71:MET:HG2 | 3:ED:309:MET:CE | 2.51 | 0.40 |
| 2:EC:912:ILE:HD11 | 3:ED:329:ASN:HB2 | 2.03 | 0.40 |
| 3:EE:114:CYS:HA | 3:EE:120:ASN:ND2 | 2.35 | 0.40 |
| 5:EI:81:LEU:HD22 | 5:EI:143:TRP:CZ3 | 2.56 | 0.40 |
| 5:EI:153:LYS:HG2 | 5:EI:154:ILE:N | 2.36 | 0.40 |
| 2:EC:1000:THR:HG21 | 5:EI:15:THR:O | 2.21 | 0.40 |
| 5:EI:234:GLN:HE22 | 7:FG:9:VAL:CG2 | 2.29 | 0.40 |
| 5:EJ:338:ASP:HB3 | 5:EJ:349:TRP:CD1 | 2.56 | 0.40 |
| 5:EJ:320:LEU:HB3 | 5:EJ:358:VAL:HB | 2.03 | 0.40 |
| 5:EJ:492:GLU:O | 5:EJ:514:HIS:HE1 | 2.04 | 0.40 |
| 4:F:149:ARG:HB3 | 4:H:168:PHE:CE1 | 2.57 | 0.40 |
| 4:F:65:GLY:HA3 | 4:F:84:ARG:NH1 | 2.36 | 0.40 |
| 5:FA:97:ASP:OD1 | 5:FA:102:TRP:CE2 | 2.74 | 0.40 |
| 5:FA:170:GLU:HA | 5:FA:238:ILE:HG13 | 2.04 | 0.40 |
| 5:FA:49:TRP:CD1 | 5:FA:67:SER:HB3 | 2.57 | 0.40 |
| 7:FE:212:PRO:HA | 7:FE:215:PHE:HB3 | 2.02 | 0.40 |
| 7:FE:51:SER:HB3 | 7:FE:54:THR:HB | 2.03 | 0.40 |
| 7:FF:520:ASN:ND2 | 7:FG:434:VAL:HG21 | 2.35 | 0.40 |
| 7:FF:250:LEU:HD23 | 7:FG:253:ARG:HH11 | 1.86 | 0.40 |
| 8:FH:85:PHE:CE2 | 8:FH:155:VAL:HG21 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:147:THR:HB | 4:G:163:SER:OG | 2.22 | 0.40 |
| 1:GD:59:LEU:CD1 | 1:GE:37:LEU:HD12 | 2.51 | 0.40 |
| 1:GD:99:LEU:O | 1:GD:99:LEU:HD12 | 2.21 | 0.40 |
| 1:GE:22:VAL:HG12 | 1:GE:23:GLY:N | 2.36 | 0.40 |
| 2:GF:145:ALA:HB2 | 2:GF:542:THR:CB | 2.48 | 0.40 |
| 2:GF:300:LEU:N | 2:GF:301:PRO:CD | 2.84 | 0.40 |
| 2:GF:379:ILE:HD11 | 2:GF:402:GLY:H | 1.86 | 0.40 |
| 2:GF:376:PHE:HB2 | 2:GF:405:VAL:HA | 2.02 | 0.40 |
| 2:GF:417:PHE:CE1 | 2:GF:423:GLU:HG2 | 2.56 | 0.40 |
| 2:GF:196:GLU:HB3 | 2:GF:520:SER:OG | 2.21 | 0.40 |
| 2:GF:788:THR:OG1 | 2:GF:789:ALA:N | 2.54 | 0.40 |
| 2:GF:819:ARG:NH2 | 3:GH:215:GLU:OE1 | 2.52 | 0.40 |
| 4:GI:168:PHE:CZ | 4:GJ:149:ARG:HB3 | 2.56 | 0.40 |
| 2:GF:58:ASN:HD22 | 4:GJ:155:ASN:ND2 | 2.19 | 0.40 |
| 4:GI:166:SER:N | 4:HA:172:GLU:HA | 2.35 | 0.40 |
| 5:HB:258:TYR:HD1 | 5:HB:386:PHE:CE1 | 2.40 | 0.40 |
| 5:HB:289:LYS:HB2 | 5:HB:371:PHE:O | 2.21 | 0.40 |
| 5:HB:258:TYR:CE1 | 5:HB:384:THR:HG23 | 2.55 | 0.40 |
| 5:HC:258:TYR:HA | 5:HC:385:TRP:O | 2.21 | 0.40 |
| 5:HB:453:ILE:HG21 | 5:HC:453:ILE:HG23 | 2.04 | 0.40 |
| 5:HC:483:GLN:NE2 | 5:HD:492:GLU:HG2 | 2.37 | 0.40 |
| 5:HD:497:PRO:HG2 | 5:HD:498:ASN:HD22 | 1.85 | 0.40 |
| 6:HE:144:ASN:HA | 6:HE:161:LEU:HD23 | 2.03 | 0.40 |
| 6:HF:26:ASP:HB3 | 6:HF:34:SER:HA | 2.03 | 0.40 |
| 6:HF:70:ILE:HD12 | 6:HF:196:LEU:HD11 | 2.03 | 0.40 |
| 6:HG:13:ARG:HG2 | 6:HG:14:LEU:N | 2.27 | 0.40 |
| 7:HH:161:THR:H | 7:HH:164:LYS:HZ1 | 1.70 | 0.40 |
| 7:HI:351:ALA:O | 7:HI:520:ASN:ND2 | 2.55 | 0.40 |
| 5:I:138:CYS:SG | 5:I:140:PRO:HD2 | 2.62 | 0.40 |
| 5:I:271:THR:HB | 5:I:273:LYS:HG2 | 2.03 | 0.40 |
| 5:I:313:PHE:CD2 | 5:I:320:LEU:HD21 | 2.56 | 0.40 |
| 5:I:258:TYR:HD1 | 5:I:386:PHE:CE1 | 2.40 | 0.40 |
| 5:J:137:TYR:HB2 | 5:J:143:TRP:HE1 | 1.86 | 0.40 |
| 5:K:267:ASP:OD1 | 5:K:285:LEU:HB2 | 2.22 | 0.40 |
| 5:K:30:PHE:O | 5:K:31:ASP:C | 2.60 | 0.40 |
| 5:K:342:CYS:HB3 | 5:K:349:TRP:CH2 | 2.57 | 0.40 |
| 5:K:357:SER:N | 5:K:372:ASP:OD1 | 2.54 | 0.40 |
| 5:K:371:PHE:CE2 | 5:K:373:SER:N | 2.90 | 0.40 |
| 6:M:86:ASP:CG | 6:M:180:GLN:HE21 | 2.18 | 0.40 |
| 7:O:139:ASN:HB2 | 7:Q:141:VAL:HG22 | 2.03 | 0.40 |
| 7:O:457:LEU:HD23 | 7:O:477:TRP:CH2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:98:THR:O | 7:P:95:TYR:HA | 2.22 | 0.40 |
| 7:Q:32:VAL:O | 7:Q:36:ILE:HG12 | 2.20 | 0.40 |
| 9:T:75:ARG:HG3 | 10:U:123:PRO:HG3 | 2.04 | 0.40 |
| 10:U:286:VAL:HG13 | 14:YF:100[E]:LYS:HE2 | 2.03 | 0.40 |
| 10:U:286:VAL:H | 14:YE:215[E]:GLU:CD | 2.25 | 0.40 |
| 10:U:311:PHE:HB3 | 10:U:312:GLY:H | 1.44 | 0.40 |
| 11:V:23:ILE:HG22 | 11:V:24:PRO:O | 2.21 | 0.40 |
| 12:W:196:GLU:HG2 | 12:W:218:MET:O | 2.21 | 0.40 |
| 1:X:132:LEU:HD23 | 1:X:132:LEU:HA | 1.77 | 0.40 |
| 1:X:355:SER:O | 1:X:379:LYS:HD3 | 2.21 | 0.40 |
| 1:X:527:ASP:OD1 | 1:X:527:ASP:C | 2.60 | 0.40 |
| 1:Y:145:PHE:HD1 | 1:Y:169:GLN:HA | 1.87 | 0.40 |
| 1:Y:331:ILE:HA | 1:Y:331:ILE:HD13 | 1.84 | 0.40 |
| 1:Y:341:THR:OG1 | 1:Y:342:ALA:N | 2.51 | 0.40 |
| 1:Y:382:LEU:HA | 1:Y:382:LEU:HD23 | 1.78 | 0.40 |
| 1:Y:515:PHE:O | 1:Y:537:ASP:HA | 2.22 | 0.40 |
| 1:X:227:ARG:HH21 | 1:Y:81:ARG:HH21 | 1.70 | 0.40 |
| 13:YA:16[F]:GLU:OE2 | 13:YA:49[F]:THR:OG1 | 2.39 | 0.40 |
| 13:YA:187[C]:ARG:HD3 | 13:YA:187[C]:ARG:HA | 1.87 | 0.40 |
| 13:YA:209[F]:GLN:HB3 | 13:YA:211[F]:VAL:HG23 | 2.02 | 0.40 |
| 13:YA:209[D]:GLN:HB2 | 13:YA:209[D]:GLN:HE21 | 1.65 | 0.40 |
| 13:YA:24[C]:LEU:HA | 13:YA:24[C]:LEU:HD12 | 1.63 | 0.40 |
| 13:YA:277[F]:LEU:HA | 13:YA:277[F]:LEU:HD23 | 1.79 | 0.40 |
| 13:YA:396[C]:GLU:HA | 13:YC:69[C]:ILE:CD1 | 2.51 | 0.40 |
| 13:YA:399[D]:HIS:ND1 | 13:YA:417[D]:PRO:HD3 | 2.36 | 0.40 |
| 13:YA:463[B]:ILE:O | 13:YB:455[B]:LYS:HA | 2.21 | 0.40 |
| 13:YA:552[B]:GLU:HB2 | 13:YB:544[B]:TRP:HB2 | 2.03 | 0.40 |
| 13:YA:75[D]:GLY:O | 13:YC:61[D]:ILE:O | 2.40 | 0.40 |
| 13:YB:148[B]:GLN:HG3 | 13:YB:421[B]:TYR:CE1 | 2.56 | 0.40 |
| 13:YB:209[E]:GLN:HB3 | 13:YB:211[E]:VAL:HG23 | 2.03 | 0.40 |
| 13:YB:227[F]:ARG:HG2 | 13:YB:228[F]:GLU:N | 2.36 | 0.40 |
| 13:YB:370[B]:ASN:ND2 | 13:YB:372[B]:SER:HB3 | 2.30 | 0.40 |
| 13:YB:432[E]:ARG:NH1 | 13:YC:432[E]:ARG:HD2 | 2.36 | 0.40 |
| 13:YB:490[E]:VAL:HG21 | 13:YC:486[E]:GLU:HB2 | 2.02 | 0.40 |
| 13:YB:16[E]:GLU:OE2 | 13:YB:49[E]:THR:OG1 | 2.40 | 0.40 |
| 13:YB:552[D]:GLU:HB2 | 13:YB:554[D]:MET:HE1 | 2.03 | 0.40 |
| 13:YB:58[F]:ILE:CG1 | 13:YB:97[F]:LEU:HD22 | 2.50 | 0.40 |
| 13:YB:76[F]:PRO:C | 13:YB:98[F]:GLY:HA2 | 2.42 | 0.40 |
| 13:YC:148[E]:GLN:HG3 | 13:YC:421[E]:TYR:CE1 | 2.56 | 0.40 |
| 13:YC:16[B]:GLU:OE2 | 13:YC:49[B]:THR:OG1 | 2.40 | 0.40 |
| 13:YC:209[B]:GLN:HB3 | 13:YC:211[B]:VAL:HG23 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YC:393[B]:MET:O | 13:YC:400[B]:ILE:HA | 2.21 | 0.40 |
| 13:YC:399[D]:HIS:ND1 | 13:YC:417[D]:PRO:HD3 | 2.36 | 0.40 |
| 13:YC:47[D]:ILE:HG23 | 14:YF:123[D]:PRO:CG | 2.49 | 0.40 |
| 13:YB:506[C]:VAL:HA | 13:YC:498[C]:VAL:O | 2.20 | 0.40 |
| 13:YA:554[A]:MET:O | 13:YC:561[A]:SER:HA | 2.22 | 0.40 |
| 13:YA:554[D]:MET:O | 13:YC:561[D]:SER:HA | 2.22 | 0.40 |
| 10:DH:286:VAL:HG13 | 14:YD:100[F]:LYS:HE2 | 2.04 | 0.40 |
| 14:YD:16[C]:LEU:CD2 | 14:YD:29[C]:VAL:HB | 2.52 | 0.40 |
| 14:YD:367[F]:ILE:HG22 | 14:YD:367[F]:ILE:O | 2.21 | 0.40 |
| 14:YE:51[D]:MET:SD | 14:YE:108[D]:GLU:HA | 2.61 | 0.40 |
| 14:YE:136[D]:LEU:HA | 14:YE:136[D]:LEU:HD23 | 1.84 | 0.40 |
| 14:YE:212[B]:ILE:HG12 | 14:YE:228[B]:TYR:HB2 | 2.03 | 0.40 |
| 14:YE:209[A]:TYR:HB3 | 14:YE:324[A]:ILE:HG12 | 2.04 | 0.40 |
| 14:YE:38[B]:LEU:HB3 | 14:YE:346[B]:LEU:HG | 2.03 | 0.40 |
| 14:YE:367[C]:ILE:O | 14:YE:367[C]:ILE:HG22 | 2.22 | 0.40 |
| 14:YE:367[E]:ILE:HG22 | 14:YE:367[E]:ILE:O | 2.21 | 0.40 |
| 14:YE:66[C]:GLY:O | 14:YE:90[C]:CYS:HB3 | 2.21 | 0.40 |
| 14:YF:228[E]:TYR:HA | 14:YF:229[E]:PRO:HD3 | 1.92 | 0.40 |
| 14:YF:360[A]:ASN:N | 14:YF:360[A]:ASN:ND2 | 2.68 | 0.40 |
| 14:YF:367[B]:ILE:O | 14:YF:367[B]:ILE:HG22 | 2.21 | 0.40 |
| 2:Z:253:ILE:HG13 | 2:Z:300:LEU:CD2 | 2.51 | 0.40 |
| 2:Z:374:LYS:HE3 | 2:Z:374:LYS:HB2 | 1.85 | 0.40 |
| 2:Z:447:ASN:OD1 | 2:Z:448:PHE:N | 2.54 | 0.40 |
| 1:A:178:ILE:HD11 | 1:A:265:ASN:O | 2.21 | 0.40 |
| 1:A:324:ARG:NH1 | 1:A:350:SER:OG | 2.48 | 0.40 |
| 1:A:472:ASP:O | 1:A:474:SER:N | 2.54 | 0.40 |
| 4:AB:145:LYS:O | 4:AB:164:ILE:HA | 2.22 | 0.40 |
| 5:AD:258:TYR:CG | 5:AD:259:THR:N | 2.90 | 0.40 |
| 5:AD:320:LEU:HB3 | 5:AD:358:VAL:HB | 2.03 | 0.40 |
| 5:AD:320:LEU:HD23 | 5:AD:358:VAL:CG2 | 2.49 | 0.40 |
| 5:AE:191:ILE:O | 5:AE:192:ARG:NH2 | 2.46 | 0.40 |
| 5:AE:371:PHE:CE2 | 5:AE:373:SER:N | 2.90 | 0.40 |
| 6:AH:79:PRO:HD2 | 6:AH:193:TRP:CB | 2.51 | 0.40 |
| 5:AC:318:GLN:HE22 | 6:AH:7:LYS:HB3 | 1.86 | 0.40 |
| 7:AI:199:VAL:HG21 | 7:AI:214:THR:HB | 2.04 | 0.40 |
| 7:AI:216:MET:HG3 | 7:AI:217:ASN:N | 2.36 | 0.40 |
| 7:AI:259:MET:HG2 | 7:AI:260:ARG:O | 2.21 | 0.40 |
| 7:AJ:223:GLU:HG3 | 7:AJ:224:TYR:CE1 | 2.57 | 0.40 |
| 7:AJ:422:LYS:HB3 | 7:BA:504:ARG:HA | 2.04 | 0.40 |
| 7:AJ:63:GLU:O | 7:AJ:66:VAL:HG22 | 2.21 | 0.40 |
| 1:B:189:ASP:O | 1:B:192:ILE:HG23 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:244:SER:O | 1:B:253:THR:OG1 | 2.34 | 0.40 |
| 1:B:382:LEU:HD12 | 1:B:647:ARG:HH12 | 1.85 | 0.40 |
| 1:B:414:LEU:O | 1:B:415:PHE:HD1 | 2.04 | 0.40 |
| 1:B:543:THR:HG1 | 1:B:544:ASP:N | 2.20 | 0.40 |
| 1:B:647:ARG:HB3 | 1:B:650:TYR:CE2 | 2.57 | 0.40 |
| 7:BA:146:SER:HB3 | 7:BA:148:PRO:HD2 | 2.04 | 0.40 |
| 7:AJ:397:GLY:N | 7:BA:402:GLY:O | 2.50 | 0.40 |
| 8:BC:49:ILE:HG23 | 8:BC:60:VAL:O | 2.21 | 0.40 |
| 11:BF:107:ASP:HA | 11:BF:155:THR:CG2 | 2.51 | 0.40 |
| 11:BF:50:ILE:HD11 | 11:BF:169:ILE:CD1 | 2.51 | 0.40 |
| 12:BG:171:TYR:HD1 | 12:BG:239:PHE:CE2 | 2.38 | 0.40 |
| 1:BH:178:ILE:HD11 | 1:BH:265:ASN:O | 2.21 | 0.40 |
| 1:BH:79:PHE:O | 1:BH:82:THR:OG1 | 2.40 | 0.40 |
| 1:BI:270:ILE:HG21 | 1:BI:270:ILE:HD13 | 1.79 | 0.40 |
| 1:BI:351:GLU:OE1 | 1:BI:351:GLU:N | 2.48 | 0.40 |
| 1:BI:378:PRO:HG2 | 1:BI:381:GLY:O | 2.21 | 0.40 |
| 1:BI:492:TYR:CD2 | 1:BI:493:LYS:HG3 | 2.57 | 0.40 |
| 2:BJ:103:PHE:H | 2:BJ:103:PHE:HD2 | 1.66 | 0.40 |
| 2:BJ:425:ARG:NH2 | 2:BJ:449:LYS:HG2 | 2.36 | 0.40 |
| 2:BJ:454:ASN:HB2 | 2:BJ:471:VAL:CG2 | 2.52 | 0.40 |
| 2:BJ:59:LEU:HA | 2:BJ:59:LEU:HD23 | 1.85 | 0.40 |
| 2:BJ:793:CYS:HA | 2:BJ:815:ASN:O | 2.22 | 0.40 |
| 2:BJ:861:TYR:HE2 | 2:BJ:863:VAL:HG22 | 1.86 | 0.40 |
| 2:BJ:884:HIS:CG | 2:BJ:885:PRO:HD2 | 2.56 | 0.40 |
| 2:BJ:958:MET:O | 2:BJ:961:VAL:HG23 | 2.21 | 0.40 |
| 2:C:223:LYS:O | 2:C:225:PHE:N | 2.55 | 0.40 |
| 2:C:454:ASN:HB2 | 2:C:471:VAL:CG2 | 2.52 | 0.40 |
| 2:C:589:LYS:HD2 | 2:C:590:ALA:H | 1.86 | 0.40 |
| 2:C:584:GLY:CA | 2:C:600:PHE:HB3 | 2.48 | 0.40 |
| 4:CE:145:LYS:O | 4:CE:164:ILE:HA | 2.22 | 0.40 |
| 5:CF:279:SER:HB2 | 5:CH:326:MET:HB2 | 2.03 | 0.40 |
| 5:CF:7:ILE:HG22 | 5:CF:8:GLY:O | 2.22 | 0.40 |
| 5:CG:170:GLU:C | 5:CG:172:GLN:H | 2.25 | 0.40 |
| 5:CG:320:LEU:HD23 | 5:CG:358:VAL:CG2 | 2.49 | 0.40 |
| 5:CG:496:ASP:OD2 | 5:CG:499:PHE:HB2 | 2.22 | 0.40 |
| 5:CH:285:LEU:CD2 | 5:CH:375:PHE:H | 2.35 | 0.40 |
| 3:D:38:PHE:HE1 | 3:D:80:LYS:HG3 | 1.86 | 0.40 |
| 7:DB:17:LYS:H | 7:DD:11:ASN:HB2 | 1.87 | 0.40 |
| 7:DB:501:THR:HB | 7:DD:422:LYS:NZ | 2.37 | 0.40 |
| 7:DB:265:LEU:N | 7:DC:256:THR:O | 2.45 | 0.40 |
| 7:DC:351:ALA:O | 7:DC:520:ASN:ND2 | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:DB:520:ASN:ND2 | 7:DC:434:VAL:HG21 | 2.36 | 0.40 |
| 7:DD:146:SER:HB3 | 7:DD:148:PRO:HD2 | 2.04 | 0.40 |
| 7:DC:190:VAL:HG12 | 7:DD:190:VAL:HG13 | 2.03 | 0.40 |
| 7:DD:417:ASN:O | 7:DD:424:ARG:NH1 | 2.54 | 0.40 |
| 8:BB:64:ARG:HD2 | 8:DE:94:GLY:O | 2.21 | 0.40 |
| 9:DG:59:ASP:O | 9:DG:63:GLU:N | 2.55 | 0.40 |
| 11:DI:146:TYR:HE2 | 11:DI:150:LEU:HD23 | 1.86 | 0.40 |
| 11:DI:50:ILE:HD11 | 11:DI:169:ILE:CD1 | 2.51 | 0.40 |
| 11:DI:64:TYR:OH | 11:DI:172:ILE:O | 2.30 | 0.40 |
| 1:EB:145:PHE:HD1 | 1:EB:169:GLN:HA | 1.87 | 0.40 |
| 1:EB:414:LEU:O | 1:EB:415:PHE:HD1 | 2.04 | 0.40 |
| 1:EB:453:GLU:O | 1:EB:454:ILE:C | 2.60 | 0.40 |
| 1:EB:515:PHE:O | 1:EB:537:ASP:HA | 2.21 | 0.40 |
| 2:EC:196:GLU:HB3 | 2:EC:520:SER:OG | 2.21 | 0.40 |
| 2:EC:223:LYS:C | 2:EC:225:PHE:H | 2.25 | 0.40 |
| 2:EC:340:PRO:C | 2:EC:342:SER:H | 2.25 | 0.40 |
| 2:EC:425:ARG:NH2 | 2:EC:449:LYS:HG2 | 2.36 | 0.40 |
| 2:EC:484:HIS:O | 2:EC:485:TYR:HB3 | 2.21 | 0.40 |
| 2:EC:577:GLY:N | 2:EC:606:ASP:O | 2.54 | 0.40 |
| 1:EA:75:VAL:HG22 | 2:EC:689:LEU:HD12 | 2.04 | 0.40 |
| 2:EC:767:GLU:O | 2:EC:845:LYS:HB2 | 2.22 | 0.40 |
| 3:EE:47:TRP:NE1 | 3:EE:270:ARG:HD2 | 2.37 | 0.40 |
| 4:EF:168:PHE:CE1 | 4:EG:161:ASN:HB3 | 2.56 | 0.40 |
| 4:EF:32:ASN:O | 4:EF:36:ASN:ND2 | 2.55 | 0.40 |
| 4:EG:147:THR:HB | 4:EG:163:SER:OG | 2.22 | 0.40 |
| 4:EG:50:VAL:O | 4:EG:52:ASN:N | 2.54 | 0.40 |
| 4:EG:63:ALA:HB3 | 4:EH:83:THR:HA | 2.04 | 0.40 |
| 5:EI:6:ASN:ND2 | 5:EI:17:ASP:OD1 | 2.55 | 0.40 |
| 5:EI:313:PHE:CD2 | 5:EI:320:LEU:HD21 | 2.56 | 0.40 |
| 7:Q:495:GLN:HA | 5:EI:425:PHE:HD2 | 1.86 | 0.40 |
| 5:EJ:104:VAL:HG13 | 5:EJ:105:ASN:N | 2.37 | 0.40 |
| 5:EJ:1:MET:H3 | 5:FA:41:ASP:HB3 | 1.87 | 0.40 |
| 5:EI:590:GLN:OE1 | 5:EJ:589:ILE:HA | 2.22 | 0.40 |
| 5:FA:181:PHE:N | 5:FA:181:PHE:CD1 | 2.88 | 0.40 |
| 6:FC:200:THR:HA | 6:FC:211:VAL:HA | 2.03 | 0.40 |
| 6:FD:70:ILE:HD12 | 6:FD:196:LEU:HD11 | 2.03 | 0.40 |
| 7:FF:194:ALA:O | 7:FF:214:THR:HG21 | 2.22 | 0.40 |
| 7:FG:147:LEU:HB2 | 7:FG:148:PRO:HD3 | 2.02 | 0.40 |
| 7:FF:480:ARG:HD3 | 7:FG:462:ASN:ND2 | 2.37 | 0.40 |
| 7:FE:443:SER:HA | 7:FG:509:GLY:O | 2.21 | 0.40 |
| 8:FH:10:PHE:CD2 | 8:FH:15:PHE:CE1 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:FI:10:PHE:CD2 | 8:FI:15:PHE:CE1 | 3.10 | 0.40 |
| 4:G:216:THR:HG23 | 4:H:222:LEU:HD13 | 2.03 | 0.40 |
| 4:G:35:PHE:CD1 | 4:G:39:TYR:HE2 | 2.39 | 0.40 |
| 4:F:64:THR:N | 4:G:82:GLY:O | 2.38 | 0.40 |
| 11:GB:107:ASP:HA | 11:GB:155:THR:CG2 | 2.51 | 0.40 |
| 1:GD:10:LEU:O | 1:GD:11:THR:OG1 | 2.31 | 0.40 |
| 1:GD:485:VAL:HG22 | 1:GD:624:TYR:CD1 | 2.53 | 0.40 |
| 1:GD:527:ASP:C | 1:GD:527:ASP:OD1 | 2.60 | 0.40 |
| 1:GE:145:PHE:HD1 | 1:GE:169:GLN:HA | 1.87 | 0.40 |
| 1:GE:143:TYR:CE2 | 1:GE:279:ASP:HB2 | 2.57 | 0.40 |
| 1:GE:322:ILE:HG13 | 1:GE:323:GLU:N | 2.35 | 0.40 |
| 2:GF:152:GLN:OE1 | 2:GF:152:GLN:N | 2.31 | 0.40 |
| 2:GF:425:ARG:NH2 | 2:GF:449:LYS:HG2 | 2.36 | 0.40 |
| 2:GF:548:ILE:O | 2:GF:555:ARG:NH2 | 2.54 | 0.40 |
| 2:GF:573:VAL:CG2 | 2:GF:610:ILE:HB | 2.51 | 0.40 |
| 2:GF:627:GLU:HB2 | 2:GF:628:HIS:CD2 | 2.56 | 0.40 |
| 2:GF:668:CYS:O | 2:GF:671:TYR:HB3 | 2.22 | 0.40 |
| 1:GE:568:ASN:HD21 | 2:GF:806:LYS:HA | 1.86 | 0.40 |
| 2:GF:852:ILE:HG21 | 2:GF:854:TYR:CZ | 2.57 | 0.40 |
| 2:GF:904:LEU:HD12 | 2:GF:905:THR:N | 2.36 | 0.40 |
| 3:GG:197:ASP:OD1 | 3:GG:197:ASP:N | 2.54 | 0.40 |
| 2:EC:528:ASN:ND2 | 3:GG:285:PRO:HB2 | 2.37 | 0.40 |
| 4:GJ:35:PHE:HB3 | 4:GJ:39:TYR:CE2 | 2.57 | 0.40 |
| 4:HA:35:PHE:HB3 | 4:HA:39:TYR:CE2 | 2.57 | 0.40 |
| 5:HB:153:LYS:HG2 | 5:HB:154:ILE:N | 2.36 | 0.40 |
| 5:HB:304:ILE:HD12 | 5:HB:384:THR:O | 2.21 | 0.40 |
| 5:HB:7:ILE:HG22 | 5:HB:8:GLY:O | 2.22 | 0.40 |
| 5:HC:552:VAL:HG22 | 5:HC:553:GLY:N | 2.36 | 0.40 |
| 5:HD:177:PHE:O | 5:HD:230:ILE:HG13 | 2.20 | 0.40 |
| 5:HD:267:ASP:OD1 | 5:HD:285:LEU:HB2 | 2.22 | 0.40 |
| 5:HD:321:ALA:O | 5:HD:324:VAL:HG12 | 2.22 | 0.40 |
| 6:HE:26:ASP:HB3 | 6:HE:34:SER:HA | 2.04 | 0.40 |
| 6:HE:13:ARG:NH1 | 6:HG:47:PHE:CZ | 2.88 | 0.40 |
| 7:HH:160:MET:HA | 7:HH:164:LYS:HZ1 | 1.86 | 0.40 |
| 7:HH:52:SER:N | 7:HJ:60:ILE:HG22 | 2.37 | 0.40 |
| 7:HI:223:GLU:HG3 | 7:HI:224:TYR:CE1 | 2.57 | 0.40 |
| 7:HH:315:ILE:O | 7:HI:321:MET:HA | 2.21 | 0.40 |
| 5:I:128:VAL:HB | 5:I:131:SER:OG | 2.21 | 0.40 |
| 8:IB:121:LYS:HG2 | 8:IB:122:THR:N | 2.37 | 0.40 |
| 10:ID:221:ALA:O | 10:ID:225:ILE:N | 2.46 | 0.40 |
| 5:J:104:VAL:HG22 | 5:J:105:ASN:N | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:J:313:PHE:CE2 | 5:J:320:LEU:HD11 | 2.57 | 0.40 |
| 5:J:89:TYR:HA | 5:J:137:TYR:CD2 | 2.57 | 0.40 |
| 5:K:170:GLU:HA | 5:K:238:ILE:HG13 | 2.04 | 0.40 |
| 5:K:303:PRO:HD2 | 5:K:365:ILE:HD13 | 2.02 | 0.40 |
| 5:K:285:LEU:CD2 | 5:K:375:PHE:H | 2.35 | 0.40 |
| 5:K:506:LEU:HD22 | 5:K:510:GLY:O | 2.22 | 0.40 |
| 6:M:200:THR:HA | 6:M:211:VAL:HA | 2.03 | 0.40 |
| 6:N:117:THR:H | 6:N:120:MET:HE3 | 1.86 | 0.40 |
| 6:N:85:THR:HG22 | 6:N:183:ILE:HD12 | 2.04 | 0.40 |
| 6:N:201:VAL:N | 6:N:210:THR:O | 2.31 | 0.40 |
| 7:O:19:ASP:HB3 | 7:Q:33:GLN:OE1 | 2.21 | 0.40 |
| 7:O:227:VAL:HG23 | 7:P:225:LYS:HB3 | 2.04 | 0.40 |
| 7:P:453:GLU:HG3 | 7:P:475:LEU:HD21 | 2.04 | 0.40 |
| 7:O:444:TYR:HB2 | 7:Q:486:ASP:HB2 | 2.02 | 0.40 |
| 8:R:22:GLN:OE1 | 8:R:116:TYR:OH | 2.25 | 0.40 |
| 11:V:9:ILE:HG12 | 11:V:10:GLU:O | 2.21 | 0.40 |
| 1:X:178:ILE:HD12 | 1:X:178:ILE:HA | 1.84 | 0.40 |
| 1:X:418:THR:HG22 | 1:X:482:ILE:HG22 | 2.02 | 0.40 |
| 7:Q:22:ASP:OD2 | 1:X:52:ARG:HD3 | 265.72 | 0.40 |
| 1:X:580:LEU:C | 1:X:580:LEU:HD12 | 2.41 | 0.40 |
| 1:Y:189:ASP:O | 1:Y:192:ILE:HG23 | 2.20 | 0.40 |
| 1:Y:143:TYR:CE2 | 1:Y:279:ASP:HB2 | 2.57 | 0.40 |
| 1:X:227:ARG:NH2 | 1:Y:81:ARG:HH21 | 2.20 | 0.40 |
| 13:YA:180[B]:LEU:HA | 13:YA:180[B]:LEU:HD13 | 1.75 | 0.40 |
| 13:YA:227[D]:ARG:HG2 | 13:YA:228[D]:GLU:N | 2.36 | 0.40 |
| 13:YA:236[B]:ILE:HG22 | 13:YA:237[B]:THR:O | 2.22 | 0.40 |
| 13:YA:236[E]:ILE:HG22 | 13:YA:237[E]:THR:O | 2.22 | 0.40 |
| 13:YA:266[A]:TRP:NE1 | 13:YA:274[A]:GLN:HG2 | 2.36 | 0.40 |
| 13:YA:393[A]:MET:O | 13:YA:400[A]:ILE:HA | 2.22 | 0.40 |
| 13:YA:453[E]:ASP:O | 13:YB:445[E]:ASP:HA | 2.22 | 0.40 |
| 13:YA:61[B]:ILE:HG12 | 13:YB:60[B]:PRO:CD | 2.51 | 0.40 |
| 13:YA:90[C]:TRP:O | 13:YA:92[C]:THR:HG23 | 2.21 | 0.40 |
| 13:YB:131[A]:VAL:O | 13:YB:134[A]:GLN:N | 2.46 | 0.40 |
| 13:YB:131[C]:VAL:O | 13:YB:134[C]:GLN:N | 2.47 | 0.40 |
| 13:YB:148[A]:GLN:HG3 | 13:YB:421[A]:TYR:CE1 | 2.56 | 0.40 |
| 13:YB:236[F]:ILE:HG22 | 13:YB:237[F]:THR:O | 2.22 | 0.40 |
| 13:YB:266[D]:TRP:NE1 | 13:YB:274[D]:GLN:HG2 | 2.36 | 0.40 |
| 13:YB:336[A]:LEU:HA | 13:YB:336[A]:LEU:HD12 | 1.85 | 0.40 |
| 13:YB:432[F]:ARG:NH1 | 13:YC:432[F]:ARG:HD2 | 2.36 | 0.40 |
| 13:YA:453[D]:ASP:O | 13:YB:445[D]:ASP:HA | 2.21 | 0.40 |
| 13:YB:471[F]:LEU:O | 13:YC:463[F]:ILE:HA | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:YA:552[C]:GLU:HB2 | 13:YB:544[C]:TRP:HB2 | 2.03 | 0.40 |
| 13:YB:552[B]:GLU:HB2 | 13:YB:554[B]:MET:HE1 | 2.03 | 0.40 |
| 13:YC:148[A]:GLN:HG3 | 13:YC:421[A]:TYR:CE1 | 2.56 | 0.40 |
| 13:YC:24[B]:LEU:HD12 | 13:YC:24[B]:LEU:HA | 1.62 | 0.40 |
| 13:YC:266[D]:TRP:NE1 | 13:YC:274[D]:GLN:HG2 | 2.36 | 0.40 |
| 13:YC:266[B]:TRP:NE1 | 13:YC:274[B]:GLN:HG2 | 2.36 | 0.40 |
| 13:YC:393[E]:MET:O | 13:YC:400[E]:ILE:HA | 2.21 | 0.40 |
| 13:YC:148[F]:GLN:HG3 | 13:YC:421[F]:TYR:CE1 | 2.56 | 0.40 |
| 13:YB:432[D]:ARG:NH1 | 13:YC:432[D]:ARG:HD2 | 2.37 | 0.40 |
| 13:YB:450[B]:VAL:HG11 | 13:YC:446[B]:GLY:H | 1.85 | 0.40 |
| 13:YB:558[B]:SER:N | 13:YC:550[B]:TRP:O | 2.47 | 0.40 |
| 14:YD:136[A]:LEU:HD21 | 14:YD:166[A]:PHE:CE2 | 2.56 | 0.40 |
| 14:YD:184[D]:LYS:HD2 | 14:YD:200[D]:TYR:HB3 | 2.04 | 0.40 |
| 14:YD:209[A]:TYR:HB3 | 14:YD:324[A]:ILE:HG12 | 2.04 | 0.40 |
| 14:YD:16[A]:LEU:CD2 | 14:YD:29[A]:VAL:HB | 2.51 | 0.40 |
| 14:YD:318[A]:LEU:HA | 14:YD:318[A]:LEU:HD12 | 1.90 | 0.40 |
| 14:YD:367[A]:ILE:O | 14:YD:367[A]:ILE:HG22 | 2.21 | 0.40 |
| 14:YD:66[E]:GLY:O | 14:YD:90[E]:CYS:HB3 | 2.22 | 0.40 |
| 10:DH:287:VAL:O | 14:YE:100[D]:LYS:HD3 | 2.21 | 0.40 |
| 14:YE:170[B]:LEU:HA | 14:YE:170[B]:LEU:HD23 | 1.69 | 0.40 |
| 14:YE:200[C]:TYR:CE1 | 14:YE:204[C]:ILE:HD11 | 2.57 | 0.40 |
| 11:BF:178:ASN:HB3 | 14:YE:217[A]:SER:H | 1.87 | 0.40 |
| 14:YE:243[A]:HIS:HD2 | 14:YF:115[A]:ILE:O | 2.03 | 0.40 |
| 14:YE:318[E]:LEU:HD12 | 14:YE:318[E]:LEU:HA | 1.90 | 0.40 |
| 14:YE:38[D]:LEU:HB3 | 14:YE:346[D]:LEU:HG | 2.03 | 0.40 |
| 14:YF:136[C]:LEU:HD21 | 14:YF:166[C]:PHE:CE2 | 2.56 | 0.40 |
| 14:YF:209[C]:TYR:HB3 | 14:YF:324[C]:ILE:HG12 | 2.04 | 0.40 |
| 14:YF:279[D]:ARG:HA | 14:YF:279[D]:ARG:HD3 | 1.44 | 0.40 |
| 14:YF:16[F]:LEU:CD2 | 14:YF:29[F]:VAL:HB | 2.52 | 0.40 |
| 14:YF:209[F]:TYR:HB3 | 14:YF:324[F]:ILE:HG12 | 2.03 | 0.40 |
| 14:YD:101[E]:GLY:HA3 | 14:YF:330[E]:LYS:HG2 | 2.03 | 0.40 |
| 14:YF:38[C]:LEU:HB3 | 14:YF:346[C]:LEU:HG | 2.03 | 0.40 |
| 14:YF:373[E]:LYS:HE2 | 14:YF:373[E]:LYS:HB3 | 1.87 | 0.40 |
| 14:YF:66[D]:GLY:O | 14:YF:90[D]:CYS:HB3 | 2.21 | 0.40 |
| 2:Z:371:ILE:HD12 | 2:Z:371:ILE:HA | 1.92 | 0.40 |
| 2:Z:454:ASN:HB2 | 2:Z:471:VAL:CG2 | 2.52 | 0.40 |
| 2:Z:821:ILE:O | 2:Z:824:GLN:NE2 | 2.32 | 0.40 |
| 2:Z:958:MET:O | 2:Z:961:VAL:HG23 | 2.21 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | B | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 1 | BH | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | BI | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 1 | EA | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | EB | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 1 | GD | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | GE | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 1 | X | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | Y | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 1 | u | 656/660 (99%) | 616 (94%) | 37 (6%) | 3 (0%) | 34 | 76 |
| 1 | v | 646/660 (98%) | 602 (93%) | 39 (6%) | 5 (1%) | 24 | 69 |
| 2 | BJ | 1000/1032 (97%) | 836 (84%) | 144 (14%) | 20 (2%) | 9 | 54 |
| 2 | C | 1000/1032 (97%) | 836 (84%) | 145 (14%) | 19 (2%) | 10 | 54 |
| 2 | EC | 1000/1032 (97%) | 836 (84%) | 145 (14%) | 19 (2%) | 10 | 54 |
| 2 | GF | 1000/1032 (97%) | 836 (84%) | 144 (14%) | 20 (2%) | 9 | 54 |
| 2 | Z | 1000/1032 (97%) | 837 (84%) | 144 (14%) | 19 (2%) | 10 | 54 |
| 2 | w | 1000/1032 (97%) | 837 (84%) | 143 (14%) | 20 (2%) | 9 | 54 |
| 3 | CA | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |
| 3 | CB | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 3 | D | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |
| 3 | E | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 3 | ED | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |
| 3 | EE | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 3 | GG | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | GH | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 3 | a | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |
| 3 | b | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 3 | x | 326/334 (98%) | 312 (96%) | 12 (4%) | 2 (1%) | 30 | 73 |
| 3 | y | 330/334 (99%) | 310 (94%) | 20 (6%) | 0 | 100 | 100 |
| 4 | AA | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | AB | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | CC | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | CD | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | CE | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | EF | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | EG | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | EH | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | F | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | G | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | GI | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | GJ | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | H | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | HA | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | c | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | d | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | e | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 4 | z | 286/288 (99%) | 271 (95%) | 11 (4%) | 4 (1%) | 14 | 59 |
| 5 | AC | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 | 61 |
| 5 | AD | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 | 55 |
| 5 | AE | 600/602 (100%) | 530 (88%) | 57 (10%) | 13 (2%) | 8 | 51 |
| 5 | CF | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 | 61 |
| 5 | CG | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 | 55 |
| 5 | CH | 600/602 (100%) | 530 (88%) | 57 (10%) | 13 (2%) | 8 | 51 |
| 5 | EI | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 | 61 |
| 5 | EJ | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 | 55 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 5 | FA | 600/602 (100%) | 530 (88%) | 57 (10%) | 13 (2%) | 8 51 |
| 5 | HB | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 61 |
| 5 | HC | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 55 |
| 5 | HD | 600/602 (100%) | 530 (88%) | 58 (10%) | 12 (2%) | 9 54 |
| 5 | I | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 61 |
| 5 | J | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 55 |
| 5 | K | 600/602 (100%) | 530 (88%) | 57 (10%) | 13 (2%) | 8 51 |
| 5 | f | 600/602 (100%) | 549 (92%) | 43 (7%) | 8 (1%) | 15 61 |
| 5 | g | 600/602 (100%) | 538 (90%) | 51 (8%) | 11 (2%) | 11 55 |
| 5 | h | 600/602 (100%) | 530 (88%) | 57 (10%) | 13 (2%) | 8 51 |
| 6 | AF | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | AG | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | AH | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | CI | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | CJ | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | DA | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | FB | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | FC | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | FD | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | HE | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | HF | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | HG | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | L | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | M | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | N | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | i | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | j | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 6 | k | 216/219 (99%) | 204 (94%) | 10 (5%) | 2 (1%) | 21 67 |
| 7 | AI | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 64 |
| 7 | AJ | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 73 |
| 7 | BA | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 61 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 7 | DB | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 | 64 |
| 7 | DC | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 | 73 |
| 7 | DD | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 | 61 |
| 7 | FE | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 | 64 |
| 7 | FF | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 | 73 |
| 7 | FG | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 | 61 |
| 7 | HH | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 | 64 |
| 7 | HI | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 | 73 |
| 7 | HJ | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 | 61 |
| 7 | O | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 | 64 |
| 7 | P | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 | 73 |
| 7 | Q | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 | 61 |
| 7 | l | 524/527 (99%) | 495 (94%) | 23 (4%) | 6 (1%) | 17 | 64 |
| 7 | m | 524/527 (99%) | 493 (94%) | 28 (5%) | 3 (1%) | 30 | 73 |
| 7 | n | 524/527 (99%) | 496 (95%) | 21 (4%) | 7 (1%) | 15 | 61 |
| 8 | BB | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | BC | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | DE | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | DF | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | FH | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | FI | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | IA | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | IB | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | R | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | S | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | o | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 8 | p | 160/163 (98%) | 147 (92%) | 13 (8%) | 0 | 100 | 100 |
| 9 | BD | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |
| 9 | DG | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |
| 9 | FJ | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |
| 9 | IC | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 9 | T | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |
| 9 | q | 124/132 (94%) | 116 (94%) | 8 (6%) | 0 | 100 | 100 |
| 10 | BE | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 10 | DH | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 10 | GA | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 10 | ID | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 10 | U | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 10 | r | 155/364 (43%) | 145 (94%) | 9 (6%) | 1 (1%) | 30 | 73 |
| 11 | BF | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | DI | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | GB | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | IE | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | V | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | s | 191/196 (97%) | 175 (92%) | 16 (8%) | 0 | 100 | 100 |
| 12 | BG | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | DJ | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | GC | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | IF | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | W | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | t | 188/320 (59%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 13 | YA | 3276/575 (570%) | 3186 (97%) | 90 (3%) | 0 | 100 | 100 |
| 13 | YB | 3276/575 (570%) | 3186 (97%) | 90 (3%) | 0 | 100 | 100 |
| 13 | YC | 3276/575 (570%) | 3186 (97%) | 90 (3%) | 0 | 100 | 100 |
| 14 | YD | 2160/391 (552%) | 2070 (96%) | 84 (4%) | 6 (0%) | 46 | 82 |
| 14 | YE | 2160/391 (552%) | 2070 (96%) | 84 (4%) | 6 (0%) | 46 | 82 |
| 14 | YF | 2160/391 (552%) | 2070 (96%) | 84 (4%) | 6 (0%) | 46 | 82 |
| 15 | ZA | 564/97 (581%) | 540 (96%) | 24 (4%) | 0 | 100 | 100 |
| All | All | 69756/58591 (119%) | 64970 (93%) | 4190 (6%) | 596 (1%) | 24 | 67 |

All (596) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 343 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | F | 249 | ILE |
| 4 | G | 249 | ILE |
| 4 | H | 249 | ILE |
| 5 | I | 10 | VAL |
| 5 | I | 24 | ILE |
| 5 | I | 171 | VAL |
| 5 | J | 24 | ILE |
| 5 | J | 171 | VAL |
| 5 | K | 24 | ILE |
| 5 | K | 152 | ASP |
| 7 | O | 47 | VAL |
| 7 | P | 47 | VAL |
| 7 | Q | 47 | VAL |
| 10 | U | 286 | VAL |
| 2 | Z | 343 | PRO |
| 4 | c | 249 | ILE |
| 4 | d | 249 | ILE |
| 4 | e | 249 | ILE |
| 5 | f | 10 | VAL |
| 5 | f | 24 | ILE |
| 5 | f | 171 | VAL |
| 5 | g | 24 | ILE |
| 5 | g | 171 | VAL |
| 5 | h | 24 | ILE |
| 5 | h | 152 | ASP |
| 7 | l | 47 | VAL |
| 7 | m | 47 | VAL |
| 7 | n | 47 | VAL |
| 10 | r | 286 | VAL |
| 2 | w | 343 | PRO |
| 4 | z | 249 | ILE |
| 4 | AA | 249 | ILE |
| 4 | AB | 249 | ILE |
| 5 | AC | 10 | VAL |
| 5 | AC | 24 | ILE |
| 5 | AC | 171 | VAL |
| 5 | AD | 24 | ILE |
| 5 | AD | 171 | VAL |
| 5 | AE | 24 | ILE |
| 5 | AE | 152 | ASP |
| 7 | AI | 47 | VAL |
| 7 | AJ | 47 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | BA | 47 | VAL |
| 10 | BE | 286 | VAL |
| 2 | BJ | 343 | PRO |
| 4 | CC | 249 | ILE |
| 4 | CD | 249 | ILE |
| 4 | CE | 249 | ILE |
| 5 | CF | 10 | VAL |
| 5 | CF | 24 | ILE |
| 5 | CF | 171 | VAL |
| 5 | CG | 24 | ILE |
| 5 | CG | 171 | VAL |
| 5 | CH | 24 | ILE |
| 5 | CH | 152 | ASP |
| 7 | DB | 47 | VAL |
| 7 | DC | 47 | VAL |
| 7 | DD | 47 | VAL |
| 10 | DH | 286 | VAL |
| 2 | EC | 343 | PRO |
| 4 | EF | 249 | ILE |
| 4 | EG | 249 | ILE |
| 4 | EH | 249 | ILE |
| 5 | EI | 10 | VAL |
| 5 | EI | 24 | ILE |
| 5 | EI | 171 | VAL |
| 5 | EJ | 24 | ILE |
| 5 | EJ | 171 | VAL |
| 5 | FA | 24 | ILE |
| 5 | FA | 152 | ASP |
| 7 | FE | 47 | VAL |
| 7 | FF | 47 | VAL |
| 7 | FG | 47 | VAL |
| 10 | GA | 286 | VAL |
| 2 | GF | 343 | PRO |
| 4 | GI | 249 | ILE |
| 4 | GJ | 249 | ILE |
| 4 | HA | 249 | ILE |
| 5 | HB | 10 | VAL |
| 5 | HB | 24 | ILE |
| 5 | HB | 171 | VAL |
| 5 | HC | 24 | ILE |
| 5 | HC | 171 | VAL |
| 5 | HD | 24 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | HD | 152 | ASP |
| 7 | HH | 47 | VAL |
| 7 | HI | 47 | VAL |
| 7 | HJ | 47 | VAL |
| 10 | ID | 286 | VAL |
| 1 | B | 46 | TYR |
| 1 | B | 534 | VAL |
| 2 | C | 168 | ILE |
| 2 | C | 360 | ASN |
| 2 | C | 411 | LYS |
| 2 | C | 947 | VAL |
| 4 | F | 51 | ALA |
| 4 | G | 51 | ALA |
| 4 | H | 51 | ALA |
| 5 | J | 85 | THR |
| 5 | J | 151 | ILE |
| 5 | J | 154 | ILE |
| 5 | K | 85 | THR |
| 5 | K | 171 | VAL |
| 5 | K | 304 | ILE |
| 5 | K | 408 | VAL |
| 7 | O | 155 | ASP |
| 7 | O | 183 | ALA |
| 7 | O | 184 | THR |
| 7 | Q | 155 | ASP |
| 1 | Y | 46 | TYR |
| 1 | Y | 534 | VAL |
| 2 | Z | 168 | ILE |
| 2 | Z | 360 | ASN |
| 2 | Z | 411 | LYS |
| 2 | Z | 947 | VAL |
| 4 | c | 51 | ALA |
| 4 | d | 51 | ALA |
| 4 | e | 51 | ALA |
| 5 | g | 85 | THR |
| 5 | g | 151 | ILE |
| 5 | g | 154 | ILE |
| 5 | h | 85 | THR |
| 5 | h | 171 | VAL |
| 5 | h | 304 | ILE |
| 5 | h | 408 | VAL |
| 7 | l | 155 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | l | 183 | ALA |
| 7 | l | 184 | THR |
| 7 | n | 155 | ASP |
| 1 | v | 46 | TYR |
| 1 | v | 534 | VAL |
| 2 | w | 168 | ILE |
| 2 | w | 360 | ASN |
| 2 | w | 411 | LYS |
| 2 | w | 947 | VAL |
| 4 | z | 51 | ALA |
| 4 | AA | 51 | ALA |
| 4 | AB | 51 | ALA |
| 5 | AD | 85 | THR |
| 5 | AD | 151 | ILE |
| 5 | AD | 154 | ILE |
| 5 | AE | 85 | THR |
| 5 | AE | 171 | VAL |
| 5 | AE | 304 | ILE |
| 5 | AE | 408 | VAL |
| 7 | AI | 155 | ASP |
| 7 | AI | 183 | ALA |
| 7 | AI | 184 | THR |
| 7 | BA | 155 | ASP |
| 1 | BI | 46 | TYR |
| 1 | BI | 534 | VAL |
| 2 | BJ | 168 | ILE |
| 2 | BJ | 360 | ASN |
| 2 | BJ | 411 | LYS |
| 2 | BJ | 947 | VAL |
| 4 | CC | 51 | ALA |
| 4 | CD | 51 | ALA |
| 4 | CE | 51 | ALA |
| 5 | CG | 85 | THR |
| 5 | CG | 151 | ILE |
| 5 | CG | 154 | ILE |
| 5 | CH | 85 | THR |
| 5 | CH | 171 | VAL |
| 5 | CH | 304 | ILE |
| 5 | CH | 408 | VAL |
| 7 | DB | 155 | ASP |
| 7 | DB | 183 | ALA |
| 7 | DB | 184 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | DD | 155 | ASP |
| 1 | EB | 46 | TYR |
| 1 | EB | 534 | VAL |
| 2 | EC | 168 | ILE |
| 2 | EC | 360 | ASN |
| 2 | EC | 411 | LYS |
| 2 | EC | 947 | VAL |
| 4 | EF | 51 | ALA |
| 4 | EG | 51 | ALA |
| 4 | EH | 51 | ALA |
| 5 | EJ | 85 | THR |
| 5 | EJ | 151 | ILE |
| 5 | EJ | 154 | ILE |
| 5 | FA | 85 | THR |
| 5 | FA | 171 | VAL |
| 5 | FA | 304 | ILE |
| 5 | FA | 408 | VAL |
| 7 | FE | 155 | ASP |
| 7 | FE | 183 | ALA |
| 7 | FE | 184 | THR |
| 7 | FG | 155 | ASP |
| 1 | GE | 46 | TYR |
| 1 | GE | 534 | VAL |
| 2 | GF | 168 | ILE |
| 2 | GF | 360 | ASN |
| 2 | GF | 411 | LYS |
| 2 | GF | 947 | VAL |
| 4 | GI | 51 | ALA |
| 4 | GJ | 51 | ALA |
| 4 | HA | 51 | ALA |
| 5 | HC | 85 | THR |
| 5 | HC | 151 | ILE |
| 5 | HC | 154 | ILE |
| 5 | HD | 85 | THR |
| 5 | HD | 171 | VAL |
| 5 | HD | 304 | ILE |
| 5 | HD | 408 | VAL |
| 7 | HH | 155 | ASP |
| 7 | HH | 183 | ALA |
| 7 | HH | 184 | THR |
| 7 | HJ | 155 | ASP |
| 2 | C | 7 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 28 | VAL |
| 2 | C | 307 | ILE |
| 2 | C | 412 | THR |
| 5 | I | 86 | VAL |
| 5 | I | 104 | VAL |
| 5 | J | 86 | VAL |
| 5 | J | 104 | VAL |
| 5 | K | 86 | VAL |
| 5 | K | 104 | VAL |
| 7 | O | 176 | ILE |
| 7 | P | 155 | ASP |
| 7 | Q | 167 | GLN |
| 2 | Z | 7 | SER |
| 2 | Z | 28 | VAL |
| 2 | Z | 307 | ILE |
| 2 | Z | 412 | THR |
| 5 | f | 86 | VAL |
| 5 | f | 104 | VAL |
| 5 | g | 86 | VAL |
| 5 | g | 104 | VAL |
| 5 | h | 86 | VAL |
| 5 | h | 104 | VAL |
| 7 | l | 176 | ILE |
| 7 | m | 155 | ASP |
| 7 | n | 167 | GLN |
| 2 | w | 7 | SER |
| 2 | w | 28 | VAL |
| 2 | w | 307 | ILE |
| 2 | w | 412 | THR |
| 5 | AC | 86 | VAL |
| 5 | AC | 104 | VAL |
| 5 | AD | 86 | VAL |
| 5 | AD | 104 | VAL |
| 5 | AE | 86 | VAL |
| 5 | AE | 104 | VAL |
| 7 | AI | 176 | ILE |
| 7 | AJ | 155 | ASP |
| 7 | BA | 167 | GLN |
| 2 | BJ | 7 | SER |
| 2 | BJ | 28 | VAL |
| 2 | BJ | 307 | ILE |
| 2 | BJ | 412 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | CF | 86 | VAL |
| 5 | CF | 104 | VAL |
| 5 | CG | 86 | VAL |
| 5 | CG | 104 | VAL |
| 5 | CH | 86 | VAL |
| 5 | CH | 104 | VAL |
| 7 | DB | 176 | ILE |
| 7 | DC | 155 | ASP |
| 7 | DD | 167 | GLN |
| 2 | EC | 7 | SER |
| 2 | EC | 28 | VAL |
| 2 | EC | 307 | ILE |
| 2 | EC | 412 | THR |
| 5 | EI | 86 | VAL |
| 5 | EI | 104 | VAL |
| 5 | EJ | 86 | VAL |
| 5 | EJ | 104 | VAL |
| 5 | FA | 86 | VAL |
| 5 | FA | 104 | VAL |
| 7 | FE | 176 | ILE |
| 7 | FF | 155 | ASP |
| 7 | FG | 167 | GLN |
| 2 | GF | 7 | SER |
| 2 | GF | 28 | VAL |
| 2 | GF | 307 | ILE |
| 2 | GF | 412 | THR |
| 5 | HB | 86 | VAL |
| 5 | HB | 104 | VAL |
| 5 | HC | 86 | VAL |
| 5 | HC | 104 | VAL |
| 5 | HD | 86 | VAL |
| 5 | HD | 104 | VAL |
| 7 | HH | 176 | ILE |
| 7 | HI | 155 | ASP |
| 7 | HJ | 167 | GLN |
| 14 | YD | 313[A] | ILE |
| 14 | YD | 313[B] | ILE |
| 14 | YD | 313[C] | ILE |
| 14 | YD | 313[D] | ILE |
| 14 | YD | 313[E] | ILE |
| 14 | YD | 313[F] | ILE |
| 14 | YE | 313[A] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 313[B] | ILE |
| 14 | YE | 313[C] | ILE |
| 14 | YE | 313[D] | ILE |
| 14 | YE | 313[E] | ILE |
| 14 | YE | 313[F] | ILE |
| 14 | YF | 313[A] | ILE |
| 14 | YF | 313[B] | ILE |
| 14 | YF | 313[C] | ILE |
| 14 | YF | 313[D] | ILE |
| 14 | YF | 313[E] | ILE |
| 14 | YF | 313[F] | ILE |
| 2 | C | 707 | GLU |
| 2 | C | 959 | ALA |
| 2 | C | 977 | ILE |
| 3 | D | 103 | PRO |
| 4 | F | 15 | ILE |
| 4 | G | 15 | ILE |
| 4 | H | 15 | ILE |
| 5 | I | 85 | THR |
| 5 | I | 180 | VAL |
| 5 | J | 180 | VAL |
| 5 | J | 277 | GLU |
| 5 | J | 559 | PRO |
| 5 | K | 90 | ASN |
| 5 | K | 180 | VAL |
| 6 | L | 11 | ILE |
| 6 | M | 11 | ILE |
| 6 | N | 11 | ILE |
| 2 | Z | 707 | GLU |
| 2 | Z | 959 | ALA |
| 2 | Z | 977 | ILE |
| 3 | a | 103 | PRO |
| 4 | c | 15 | ILE |
| 4 | d | 15 | ILE |
| 4 | e | 15 | ILE |
| 5 | f | 85 | THR |
| 5 | f | 180 | VAL |
| 5 | g | 180 | VAL |
| 5 | g | 277 | GLU |
| 5 | g | 559 | PRO |
| 5 | h | 90 | ASN |
| 5 | h | 180 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | i | 11 | ILE |
| 6 | j | 11 | ILE |
| 6 | k | 11 | ILE |
| 2 | w | 707 | GLU |
| 2 | w | 959 | ALA |
| 2 | w | 977 | ILE |
| 3 | x | 103 | PRO |
| 4 | z | 15 | ILE |
| 4 | AA | 15 | ILE |
| 4 | AB | 15 | ILE |
| 5 | AC | 85 | THR |
| 5 | AC | 180 | VAL |
| 5 | AD | 180 | VAL |
| 5 | AD | 277 | GLU |
| 5 | AD | 559 | PRO |
| 5 | AE | 90 | ASN |
| 5 | AE | 180 | VAL |
| 6 | AF | 11 | ILE |
| 6 | AG | 11 | ILE |
| 6 | AH | 11 | ILE |
| 2 | BJ | 707 | GLU |
| 2 | BJ | 959 | ALA |
| 2 | BJ | 977 | ILE |
| 3 | CA | 103 | PRO |
| 4 | CC | 15 | ILE |
| 4 | CD | 15 | ILE |
| 4 | CE | 15 | ILE |
| 5 | CF | 85 | THR |
| 5 | CF | 180 | VAL |
| 5 | CG | 180 | VAL |
| 5 | CG | 277 | GLU |
| 5 | CG | 559 | PRO |
| 5 | CH | 90 | ASN |
| 5 | CH | 180 | VAL |
| 6 | CI | 11 | ILE |
| 6 | CJ | 11 | ILE |
| 6 | DA | 11 | ILE |
| 2 | EC | 707 | GLU |
| 2 | EC | 959 | ALA |
| 2 | EC | 977 | ILE |
| 3 | ED | 103 | PRO |
| 4 | EF | 15 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | EG | 15 | ILE |
| 4 | EH | 15 | ILE |
| 5 | EI | 85 | THR |
| 5 | EI | 180 | VAL |
| 5 | EJ | 180 | VAL |
| 5 | EJ | 277 | GLU |
| 5 | FA | 90 | ASN |
| 5 | FA | 180 | VAL |
| 6 | FB | 11 | ILE |
| 6 | FC | 11 | ILE |
| 6 | FD | 11 | ILE |
| 2 | GF | 707 | GLU |
| 2 | GF | 977 | ILE |
| 3 | GG | 103 | PRO |
| 4 | GI | 15 | ILE |
| 4 | GJ | 15 | ILE |
| 4 | HA | 15 | ILE |
| 5 | HB | 85 | THR |
| 5 | HB | 180 | VAL |
| 5 | HC | 180 | VAL |
| 5 | HC | 277 | GLU |
| 5 | HC | 559 | PRO |
| 5 | HD | 90 | ASN |
| 5 | HD | 180 | VAL |
| 6 | HE | 11 | ILE |
| 6 | HF | 11 | ILE |
| 6 | HG | 11 | ILE |
| 1 | A | 140 | VAL |
| 1 | A | 473 | HIS |
| 1 | B | 379 | LYS |
| 2 | C | 87 | GLN |
| 2 | C | 342 | SER |
| 2 | C | 361 | PRO |
| 4 | F | 50 | VAL |
| 4 | G | 50 | VAL |
| 4 | H | 50 | VAL |
| 5 | K | 64 | TRP |
| 5 | K | 151 | ILE |
| 6 | L | 4 | LEU |
| 6 | M | 4 | LEU |
| 6 | N | 4 | LEU |
| 7 | O | 48 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | Q | 49 | ASP |
| 7 | Q | 157 | THR |
| 1 | X | 140 | VAL |
| 1 | X | 473 | HIS |
| 1 | Y | 379 | LYS |
| 2 | Z | 87 | GLN |
| 2 | Z | 342 | SER |
| 2 | Z | 361 | PRO |
| 4 | c | 50 | VAL |
| 4 | d | 50 | VAL |
| 4 | e | 50 | VAL |
| 5 | h | 64 | TRP |
| 5 | h | 151 | ILE |
| 6 | i | 4 | LEU |
| 6 | j | 4 | LEU |
| 6 | k | 4 | LEU |
| 7 | l | 48 | PRO |
| 7 | n | 49 | ASP |
| 7 | n | 157 | THR |
| 1 | u | 140 | VAL |
| 1 | u | 473 | HIS |
| 1 | v | 379 | LYS |
| 2 | w | 87 | GLN |
| 2 | w | 342 | SER |
| 2 | w | 361 | PRO |
| 4 | z | 50 | VAL |
| 4 | AA | 50 | VAL |
| 4 | AB | 50 | VAL |
| 5 | AE | 64 | TRP |
| 5 | AE | 151 | ILE |
| 6 | AF | 4 | LEU |
| 6 | AG | 4 | LEU |
| 6 | AH | 4 | LEU |
| 7 | AI | 48 | PRO |
| 7 | BA | 49 | ASP |
| 7 | BA | 157 | THR |
| 1 | BH | 140 | VAL |
| 1 | BH | 473 | HIS |
| 1 | BI | 379 | LYS |
| 2 | BJ | 87 | GLN |
| 2 | BJ | 342 | SER |
| 2 | BJ | 361 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | CC | 50 | VAL |
| 4 | CD | 50 | VAL |
| 4 | CE | 50 | VAL |
| 5 | CH | 64 | TRP |
| 5 | CH | 151 | ILE |
| 6 | CI | 4 | LEU |
| 6 | CJ | 4 | LEU |
| 6 | DA | 4 | LEU |
| 7 | DB | 48 | PRO |
| 7 | DD | 49 | ASP |
| 7 | DD | 157 | THR |
| 1 | EA | 140 | VAL |
| 1 | EA | 473 | HIS |
| 1 | EB | 379 | LYS |
| 2 | EC | 87 | GLN |
| 2 | EC | 342 | SER |
| 2 | EC | 361 | PRO |
| 4 | EF | 50 | VAL |
| 4 | EG | 50 | VAL |
| 4 | EH | 50 | VAL |
| 5 | EJ | 559 | PRO |
| 5 | FA | 64 | TRP |
| 5 | FA | 151 | ILE |
| 6 | FB | 4 | LEU |
| 6 | FC | 4 | LEU |
| 6 | FD | 4 | LEU |
| 7 | FE | 48 | PRO |
| 7 | FG | 49 | ASP |
| 7 | FG | 157 | THR |
| 1 | GD | 473 | HIS |
| 1 | GE | 379 | LYS |
| 2 | GF | 87 | GLN |
| 2 | GF | 342 | SER |
| 2 | GF | 361 | PRO |
| 2 | GF | 959 | ALA |
| 4 | GI | 50 | VAL |
| 4 | GJ | 50 | VAL |
| 4 | HA | 50 | VAL |
| 5 | HD | 64 | TRP |
| 5 | HD | 151 | ILE |
| 6 | HE | 4 | LEU |
| 6 | HF | 4 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | HG | 4 | LEU |
| 7 | HH | 48 | PRO |
| 7 | HJ | 49 | ASP |
| 7 | HJ | 157 | THR |
| 1 | B | 454 | ILE |
| 3 | D | 102 | ASP |
| 5 | I | 228 | PHE |
| 5 | J | 90 | ASN |
| 5 | K | 156 | SER |
| 1 | Y | 454 | ILE |
| 3 | a | 102 | ASP |
| 5 | f | 228 | PHE |
| 5 | g | 90 | ASN |
| 5 | h | 156 | SER |
| 1 | v | 454 | ILE |
| 2 | w | 341 | LEU |
| 3 | x | 102 | ASP |
| 5 | AC | 228 | PHE |
| 5 | AD | 90 | ASN |
| 5 | AE | 156 | SER |
| 1 | BI | 454 | ILE |
| 2 | BJ | 341 | LEU |
| 3 | CA | 102 | ASP |
| 5 | CF | 228 | PHE |
| 5 | CG | 90 | ASN |
| 5 | CH | 156 | SER |
| 1 | EB | 454 | ILE |
| 3 | ED | 102 | ASP |
| 5 | EI | 228 | PHE |
| 5 | EJ | 90 | ASN |
| 5 | FA | 156 | SER |
| 1 | GD | 140 | VAL |
| 1 | GE | 454 | ILE |
| 2 | GF | 341 | LEU |
| 2 | GF | 992 | PRO |
| 3 | GG | 102 | ASP |
| 5 | HB | 228 | PHE |
| 5 | HC | 90 | ASN |
| 2 | C | 992 | PRO |
| 2 | Z | 992 | PRO |
| 2 | w | 992 | PRO |
| 2 | BJ | 992 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | EC | 992 | PRO |
| 2 | C | 357 | ILE |
| 2 | Z | 357 | ILE |
| 2 | w | 357 | ILE |
| 2 | BJ | 357 | ILE |
| 2 | EC | 357 | ILE |
| 2 | GF | 357 | ILE |
| 1 | B | 223 | ILE |
| 7 | P | 29 | ILE |
| 1 | Y | 223 | ILE |
| 7 | m | 29 | ILE |
| 1 | v | 223 | ILE |
| 7 | AJ | 29 | ILE |
| 1 | BI | 223 | ILE |
| 7 | DC | 29 | ILE |
| 1 | EB | 223 | ILE |
| 7 | FF | 29 | ILE |
| 1 | GE | 223 | ILE |
| 7 | HI | 29 | ILE |
| 2 | C | 842 | VAL |
| 2 | C | 1019 | PRO |
| 7 | Q | 87 | TYR |
| 2 | Z | 842 | VAL |
| 7 | n | 87 | TYR |
| 2 | w | 842 | VAL |
| 7 | BA | 87 | TYR |
| 2 | BJ | 842 | VAL |
| 2 | BJ | 1019 | PRO |
| 7 | DD | 87 | TYR |
| 2 | EC | 842 | VAL |
| 7 | FG | 87 | TYR |
| 2 | GF | 842 | VAL |
| 7 | HJ | 87 | TYR |
| 7 | Q | 29 | ILE |
| 2 | Z | 1019 | PRO |
| 7 | n | 29 | ILE |
| 2 | w | 1019 | PRO |
| 7 | BA | 29 | ILE |
| 7 | DD | 29 | ILE |
| 2 | EC | 1019 | PRO |
| 7 | FG | 29 | ILE |
| 2 | GF | 1019 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | HJ | 29 | ILE |
| 1 | A | 319 | PRO |
| 1 | X | 319 | PRO |
| 1 | u | 319 | PRO |
| 1 | BH | 319 | PRO |
| 1 | EA | 319 | PRO |
| 1 | GD | 319 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | B | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 1 | BH | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | BI | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 1 | EA | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | EB | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 1 | GD | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | GE | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 1 | X | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | Y | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 1 | u | 576/578 (100%) | 576 (100%) | 0 | 100 | 100 |
| 1 | v | 567/578 (98%) | 567 (100%) | 0 | 100 | 100 |
| 2 | BJ | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |
| 2 | C | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |
| 2 | EC | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |
| 2 | GF | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |
| 2 | Z | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |
| 2 | w | 896/921 (97%) | 896 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | CA | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | CB | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 3 | D | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | E | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 3 | ED | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | EE | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 3 | GG | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | GH | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 3 | a | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | b | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 3 | x | 289/295 (98%) | 289 (100%) | 0 | 100 | 100 |
| 3 | y | 293/295 (99%) | 293 (100%) | 0 | 100 | 100 |
| 4 | AA | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | AB | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | CC | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | CD | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | CE | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | EF | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | EG | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | EH | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | F | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | G | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | GI | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | GJ | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | H | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | HA | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | c | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | d | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | e | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 4 | z | 244/244 (100%) | 244 (100%) | 0 | 100 | 100 |
| 5 | AC | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 5 | AD | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | AE | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 5 | CF | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | CG | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | CH | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 5 | EI | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | EJ | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | FA | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 5 | HB | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | HC | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | HD | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 5 | I | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | J | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | K | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 5 | f | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | g | 519/519 (100%) | 519 (100%) | 0 | 100 | 100 |
| 5 | h | 519/519 (100%) | 518 (100%) | 1 (0%) | 95 | 97 |
| 6 | AF | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | AG | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | AH | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | CI | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | CJ | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | DA | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | FB | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | FC | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | FD | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | HE | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | HF | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | HG | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | L | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | M | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | N | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | i | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | j | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 6 | k | 187/188 (100%) | 187 (100%) | 0 | 100 | 100 |
| 7 | AI | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | AJ | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | BA | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | DB | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | DC | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | DD | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | FE | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | FF | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | FG | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | HH | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | HI | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | HJ | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | O | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | P | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | Q | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | l | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 7 | m | 426/427 (100%) | 425 (100%) | 1 (0%) | 95 | 97 |
| 7 | n | 426/427 (100%) | 426 (100%) | 0 | 100 | 100 |
| 8 | BB | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | BC | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | DE | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | DF | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | FH | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | FI | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | IA | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | IB | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | R | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 8 | S | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | o | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 8 | p | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 9 | BD | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 9 | DG | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 9 | FJ | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 9 | IC | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 9 | T | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 9 | q | 118/123 (96%) | 118 (100%) | 0 | 100 | 100 |
| 10 | BE | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 10 | DH | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 10 | GA | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 10 | ID | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 10 | U | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 10 | r | 146/313 (47%) | 145 (99%) | 1 (1%) | 88 | 94 |
| 11 | BF | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 11 | DI | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 11 | GB | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 11 | IE | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 11 | V | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 11 | s | 166/169 (98%) | 165 (99%) | 1 (1%) | 90 | 95 |
| 12 | BG | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 12 | DJ | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 12 | GC | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 12 | IF | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 12 | W | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 12 | t | 171/275 (62%) | 170 (99%) | 1 (1%) | 90 | 95 |
| 13 | YA | 2814/485 (580%) | 2544 (90%) | 270 (10%) | 10 | 44 |
| 13 | YB | 2814/485 (580%) | 2544 (90%) | 270 (10%) | 10 | 44 |
| 13 | YC | 2814/485 (580%) | 2544 (90%) | 270 (10%) | 10 | 44 |
| 14 | YD | 1944/350 (555%) | 1710 (88%) | 234 (12%) | 6 | 34 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 14 | YE | 1944/350 (555%) | 1710 (88%) | 234 (12%) | 6 34 |
| 14 | YF | 1944/350 (555%) | 1710 (88%) | 234 (12%) | 6 34 |
| 15 | ZA | 468/79 (592%) | 450 (96%) | 18 (4%) | 40 75 |
| All | All | 60474/50314 (120%) | 58914 (97%) | 1560 (3%) | 91 81 |

All (1560) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | K | 79 | ILE |
| 7 | P | 9 | VAL |
| 10 | U | 286 | VAL |
| 11 | V | 15 | THR |
| 12 | W | 199 | ILE |
| 5 | h | 79 | ILE |
| 7 | m | 9 | VAL |
| 10 | r | 286 | VAL |
| 11 | s | 15 | THR |
| 12 | t | 199 | ILE |
| 5 | AE | 79 | ILE |
| 7 | AJ | 9 | VAL |
| 10 | BE | 286 | VAL |
| 11 | BF | 15 | THR |
| 12 | BG | 199 | ILE |
| 5 | CH | 79 | ILE |
| 7 | DC | 9 | VAL |
| 10 | DH | 286 | VAL |
| 11 | DI | 15 | THR |
| 12 | DJ | 199 | ILE |
| 5 | FA | 79 | ILE |
| 7 | FF | 9 | VAL |
| 10 | GA | 286 | VAL |
| 11 | GB | 15 | THR |
| 12 | GC | 199 | ILE |
| 5 | HD | 79 | ILE |
| 7 | HI | 9 | VAL |
| 10 | ID | 286 | VAL |
| 11 | IE | 15 | THR |
| 12 | IF | 199 | ILE |
| 13 | YA | 7[A] | ASN |
| 13 | YA | 7[B] | ASN |
| 13 | YA | 7[C] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 7[D] | ASN |
| 13 | YA | 7[E] | ASN |
| 13 | YA | 7[F] | ASN |
| 13 | YA | 24[A] | LEU |
| 13 | YA | 24[B] | LEU |
| 13 | YA | 24[C] | LEU |
| 13 | YA | 24[D] | LEU |
| 13 | YA | 24[E] | LEU |
| 13 | YA | 24[F] | LEU |
| 13 | YA | 27[A] | VAL |
| 13 | YA | 27[B] | VAL |
| 13 | YA | 27[C] | VAL |
| 13 | YA | 27[D] | VAL |
| 13 | YA | 27[E] | VAL |
| 13 | YA | 27[F] | VAL |
| 13 | YA | 34[A] | LEU |
| 13 | YA | 34[B] | LEU |
| 13 | YA | 34[C] | LEU |
| 13 | YA | 34[D] | LEU |
| 13 | YA | 34[E] | LEU |
| 13 | YA | 34[F] | LEU |
| 13 | YA | 41[A] | GLN |
| 13 | YA | 41[B] | GLN |
| 13 | YA | 41[C] | GLN |
| 13 | YA | 41[D] | GLN |
| 13 | YA | 41[E] | GLN |
| 13 | YA | 41[F] | GLN |
| 13 | YA | 50[A] | GLU |
| 13 | YA | 50[B] | GLU |
| 13 | YA | 50[C] | GLU |
| 13 | YA | 50[D] | GLU |
| 13 | YA | 50[E] | GLU |
| 13 | YA | 50[F] | GLU |
| 13 | YA | 56[A] | SER |
| 13 | YA | 56[B] | SER |
| 13 | YA | 56[C] | SER |
| 13 | YA | 56[D] | SER |
| 13 | YA | 56[E] | SER |
| 13 | YA | 56[F] | SER |
| 13 | YA | 57[A] | VAL |
| 13 | YA | 57[B] | VAL |
| 13 | YA | 57[C] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 57[D] | VAL |
| 13 | YA | 57[E] | VAL |
| 13 | YA | 57[F] | VAL |
| 13 | YA | 59[A] | GLN |
| 13 | YA | 59[B] | GLN |
| 13 | YA | 59[C] | GLN |
| 13 | YA | 59[D] | GLN |
| 13 | YA | 59[E] | GLN |
| 13 | YA | 59[F] | GLN |
| 13 | YA | 61[A] | ILE |
| 13 | YA | 61[B] | ILE |
| 13 | YA | 61[C] | ILE |
| 13 | YA | 61[D] | ILE |
| 13 | YA | 61[E] | ILE |
| 13 | YA | 61[F] | ILE |
| 13 | YA | 66[A] | MET |
| 13 | YA | 66[B] | MET |
| 13 | YA | 66[C] | MET |
| 13 | YA | 66[D] | MET |
| 13 | YA | 66[E] | MET |
| 13 | YA | 66[F] | MET |
| 13 | YA | 82[A] | VAL |
| 13 | YA | 82[B] | VAL |
| 13 | YA | 82[C] | VAL |
| 13 | YA | 82[D] | VAL |
| 13 | YA | 82[E] | VAL |
| 13 | YA | 82[F] | VAL |
| 13 | YA | 87[A] | LEU |
| 13 | YA | 87[B] | LEU |
| 13 | YA | 87[C] | LEU |
| 13 | YA | 87[D] | LEU |
| 13 | YA | 87[E] | LEU |
| 13 | YA | 87[F] | LEU |
| 13 | YA | 89[A] | LYS |
| 13 | YA | 89[B] | LYS |
| 13 | YA | 89[C] | LYS |
| 13 | YA | 89[D] | LYS |
| 13 | YA | 89[E] | LYS |
| 13 | YA | 89[F] | LYS |
| 13 | YA | 97[A] | LEU |
| 13 | YA | 97[B] | LEU |
| 13 | YA | 97[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 97[D] | LEU |
| 13 | YA | 97[E] | LEU |
| 13 | YA | 97[F] | LEU |
| 13 | YA | 127[A] | ASN |
| 13 | YA | 127[B] | ASN |
| 13 | YA | 127[C] | ASN |
| 13 | YA | 127[D] | ASN |
| 13 | YA | 127[E] | ASN |
| 13 | YA | 127[F] | ASN |
| 13 | YA | 150[A] | SER |
| 13 | YA | 150[B] | SER |
| 13 | YA | 150[C] | SER |
| 13 | YA | 150[D] | SER |
| 13 | YA | 150[E] | SER |
| 13 | YA | 150[F] | SER |
| 13 | YA | 152[A] | LEU |
| 13 | YA | 152[B] | LEU |
| 13 | YA | 152[C] | LEU |
| 13 | YA | 152[D] | LEU |
| 13 | YA | 152[E] | LEU |
| 13 | YA | 152[F] | LEU |
| 13 | YA | 173[A] | ASN |
| 13 | YA | 173[B] | ASN |
| 13 | YA | 173[C] | ASN |
| 13 | YA | 173[D] | ASN |
| 13 | YA | 173[E] | ASN |
| 13 | YA | 173[F] | ASN |
| 13 | YA | 180[A] | LEU |
| 13 | YA | 180[B] | LEU |
| 13 | YA | 180[C] | LEU |
| 13 | YA | 180[D] | LEU |
| 13 | YA | 180[E] | LEU |
| 13 | YA | 180[F] | LEU |
| 13 | YA | 182[A] | ARG |
| 13 | YA | 182[B] | ARG |
| 13 | YA | 182[C] | ARG |
| 13 | YA | 182[D] | ARG |
| 13 | YA | 182[E] | ARG |
| 13 | YA | 182[F] | ARG |
| 13 | YA | 195[A] | GLU |
| 13 | YA | 195[B] | GLU |
| 13 | YA | 195[C] | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 195[D] | GLU |
| 13 | YA | 195[E] | GLU |
| 13 | YA | 195[F] | GLU |
| 13 | YA | 209[A] | GLN |
| 13 | YA | 209[B] | GLN |
| 13 | YA | 209[C] | GLN |
| 13 | YA | 209[D] | GLN |
| 13 | YA | 209[E] | GLN |
| 13 | YA | 209[F] | GLN |
| 13 | YA | 242[A] | THR |
| 13 | YA | 242[B] | THR |
| 13 | YA | 242[C] | THR |
| 13 | YA | 242[D] | THR |
| 13 | YA | 242[E] | THR |
| 13 | YA | 242[F] | THR |
| 13 | YA | 296[A] | LEU |
| 13 | YA | 296[B] | LEU |
| 13 | YA | 296[C] | LEU |
| 13 | YA | 296[D] | LEU |
| 13 | YA | 296[E] | LEU |
| 13 | YA | 296[F] | LEU |
| 13 | YA | 300[A] | LEU |
| 13 | YA | 300[B] | LEU |
| 13 | YA | 300[C] | LEU |
| 13 | YA | 300[D] | LEU |
| 13 | YA | 300[E] | LEU |
| 13 | YA | 300[F] | LEU |
| 13 | YA | 327[A] | VAL |
| 13 | YA | 327[B] | VAL |
| 13 | YA | 327[C] | VAL |
| 13 | YA | 327[D] | VAL |
| 13 | YA | 327[E] | VAL |
| 13 | YA | 327[F] | VAL |
| 13 | YA | 331[A] | ILE |
| 13 | YA | 331[B] | ILE |
| 13 | YA | 331[C] | ILE |
| 13 | YA | 331[D] | ILE |
| 13 | YA | 331[E] | ILE |
| 13 | YA | 331[F] | ILE |
| 13 | YA | 335[A] | ASN |
| 13 | YA | 335[B] | ASN |
| 13 | YA | 335[C] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 335[D] | ASN |
| 13 | YA | 335[E] | ASN |
| 13 | YA | 335[F] | ASN |
| 13 | YA | 372[A] | SER |
| 13 | YA | 372[B] | SER |
| 13 | YA | 372[C] | SER |
| 13 | YA | 372[D] | SER |
| 13 | YA | 372[E] | SER |
| 13 | YA | 372[F] | SER |
| 13 | YA | 373[A] | ARG |
| 13 | YA | 373[B] | ARG |
| 13 | YA | 373[C] | ARG |
| 13 | YA | 373[D] | ARG |
| 13 | YA | 373[E] | ARG |
| 13 | YA | 373[F] | ARG |
| 13 | YA | 375[A] | LEU |
| 13 | YA | 375[B] | LEU |
| 13 | YA | 375[C] | LEU |
| 13 | YA | 375[D] | LEU |
| 13 | YA | 375[E] | LEU |
| 13 | YA | 375[F] | LEU |
| 13 | YA | 418[A] | THR |
| 13 | YA | 418[B] | THR |
| 13 | YA | 418[C] | THR |
| 13 | YA | 418[D] | THR |
| 13 | YA | 418[E] | THR |
| 13 | YA | 418[F] | THR |
| 13 | YA | 429[A] | ARG |
| 13 | YA | 429[B] | ARG |
| 13 | YA | 429[C] | ARG |
| 13 | YA | 429[D] | ARG |
| 13 | YA | 429[E] | ARG |
| 13 | YA | 429[F] | ARG |
| 13 | YA | 432[A] | ARG |
| 13 | YA | 432[B] | ARG |
| 13 | YA | 432[C] | ARG |
| 13 | YA | 432[D] | ARG |
| 13 | YA | 432[E] | ARG |
| 13 | YA | 432[F] | ARG |
| 13 | YA | 435[A] | VAL |
| 13 | YA | 435[B] | VAL |
| 13 | YA | 435[C] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 435[D] | VAL |
| 13 | YA | 435[E] | VAL |
| 13 | YA | 435[F] | VAL |
| 13 | YA | 442[A] | THR |
| 13 | YA | 442[B] | THR |
| 13 | YA | 442[C] | THR |
| 13 | YA | 442[D] | THR |
| 13 | YA | 442[E] | THR |
| 13 | YA | 442[F] | THR |
| 13 | YA | 455[A] | LYS |
| 13 | YA | 455[B] | LYS |
| 13 | YA | 455[C] | LYS |
| 13 | YA | 455[D] | LYS |
| 13 | YA | 455[E] | LYS |
| 13 | YA | 455[F] | LYS |
| 13 | YA | 465[A] | TYR |
| 13 | YA | 465[B] | TYR |
| 13 | YA | 465[C] | TYR |
| 13 | YA | 465[D] | TYR |
| 13 | YA | 465[E] | TYR |
| 13 | YA | 465[F] | TYR |
| 13 | YA | 486[A] | GLU |
| 13 | YA | 486[B] | GLU |
| 13 | YA | 486[C] | GLU |
| 13 | YA | 486[D] | GLU |
| 13 | YA | 486[E] | GLU |
| 13 | YA | 486[F] | GLU |
| 13 | YA | 522[A] | VAL |
| 13 | YA | 522[B] | VAL |
| 13 | YA | 522[C] | VAL |
| 13 | YA | 522[D] | VAL |
| 13 | YA | 522[E] | VAL |
| 13 | YA | 522[F] | VAL |
| 13 | YA | 550[A] | TRP |
| 13 | YA | 550[B] | TRP |
| 13 | YA | 550[C] | TRP |
| 13 | YA | 550[D] | TRP |
| 13 | YA | 550[E] | TRP |
| 13 | YA | 550[F] | TRP |
| 13 | YA | 554[A] | MET |
| 13 | YA | 554[B] | MET |
| 13 | YA | 554[C] | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YA | 554[D] | MET |
| 13 | YA | 554[E] | MET |
| 13 | YA | 554[F] | MET |
| 13 | YA | 566[A] | THR |
| 13 | YA | 566[B] | THR |
| 13 | YA | 566[C] | THR |
| 13 | YA | 566[D] | THR |
| 13 | YA | 566[E] | THR |
| 13 | YA | 566[F] | THR |
| 13 | YA | 573[A] | ASP |
| 13 | YA | 573[B] | ASP |
| 13 | YA | 573[C] | ASP |
| 13 | YA | 573[D] | ASP |
| 13 | YA | 573[E] | ASP |
| 13 | YA | 573[F] | ASP |
| 13 | YB | 7[A] | ASN |
| 13 | YB | 7[B] | ASN |
| 13 | YB | 7[C] | ASN |
| 13 | YB | 7[D] | ASN |
| 13 | YB | 7[E] | ASN |
| 13 | YB | 7[F] | ASN |
| 13 | YB | 24[A] | LEU |
| 13 | YB | 24[B] | LEU |
| 13 | YB | 24[C] | LEU |
| 13 | YB | 24[D] | LEU |
| 13 | YB | 24[E] | LEU |
| 13 | YB | 24[F] | LEU |
| 13 | YB | 27[A] | VAL |
| 13 | YB | 27[B] | VAL |
| 13 | YB | 27[C] | VAL |
| 13 | YB | 27[D] | VAL |
| 13 | YB | 27[E] | VAL |
| 13 | YB | 27[F] | VAL |
| 13 | YB | 34[A] | LEU |
| 13 | YB | 34[B] | LEU |
| 13 | YB | 34[C] | LEU |
| 13 | YB | 34[D] | LEU |
| 13 | YB | 34[E] | LEU |
| 13 | YB | 34[F] | LEU |
| 13 | YB | 41[A] | GLN |
| 13 | YB | 41[B] | GLN |
| 13 | YB | 41[C] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 41[D] | GLN |
| 13 | YB | 41[E] | GLN |
| 13 | YB | 41[F] | GLN |
| 13 | YB | 50[A] | GLU |
| 13 | YB | 50[B] | GLU |
| 13 | YB | 50[C] | GLU |
| 13 | YB | 50[D] | GLU |
| 13 | YB | 50[E] | GLU |
| 13 | YB | 50[F] | GLU |
| 13 | YB | 56[A] | SER |
| 13 | YB | 56[B] | SER |
| 13 | YB | 56[C] | SER |
| 13 | YB | 56[D] | SER |
| 13 | YB | 56[E] | SER |
| 13 | YB | 56[F] | SER |
| 13 | YB | 57[A] | VAL |
| 13 | YB | 57[B] | VAL |
| 13 | YB | 57[C] | VAL |
| 13 | YB | 57[D] | VAL |
| 13 | YB | 57[E] | VAL |
| 13 | YB | 57[F] | VAL |
| 13 | YB | 59[A] | GLN |
| 13 | YB | 59[B] | GLN |
| 13 | YB | 59[C] | GLN |
| 13 | YB | 59[D] | GLN |
| 13 | YB | 59[E] | GLN |
| 13 | YB | 59[F] | GLN |
| 13 | YB | 61[A] | ILE |
| 13 | YB | 61[B] | ILE |
| 13 | YB | 61[C] | ILE |
| 13 | YB | 61[D] | ILE |
| 13 | YB | 61[E] | ILE |
| 13 | YB | 61[F] | ILE |
| 13 | YB | 66[A] | MET |
| 13 | YB | 66[B] | MET |
| 13 | YB | 66[C] | MET |
| 13 | YB | 66[D] | MET |
| 13 | YB | 66[E] | MET |
| 13 | YB | 66[F] | MET |
| 13 | YB | 82[A] | VAL |
| 13 | YB | 82[B] | VAL |
| 13 | YB | 82[C] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 82[D] | VAL |
| 13 | YB | 82[E] | VAL |
| 13 | YB | 82[F] | VAL |
| 13 | YB | 87[A] | LEU |
| 13 | YB | 87[B] | LEU |
| 13 | YB | 87[C] | LEU |
| 13 | YB | 87[D] | LEU |
| 13 | YB | 87[E] | LEU |
| 13 | YB | 87[F] | LEU |
| 13 | YB | 89[A] | LYS |
| 13 | YB | 89[B] | LYS |
| 13 | YB | 89[C] | LYS |
| 13 | YB | 89[D] | LYS |
| 13 | YB | 89[E] | LYS |
| 13 | YB | 89[F] | LYS |
| 13 | YB | 97[A] | LEU |
| 13 | YB | 97[B] | LEU |
| 13 | YB | 97[C] | LEU |
| 13 | YB | 97[D] | LEU |
| 13 | YB | 97[E] | LEU |
| 13 | YB | 97[F] | LEU |
| 13 | YB | 127[A] | ASN |
| 13 | YB | 127[B] | ASN |
| 13 | YB | 127[C] | ASN |
| 13 | YB | 127[D] | ASN |
| 13 | YB | 127[E] | ASN |
| 13 | YB | 127[F] | ASN |
| 13 | YB | 150[A] | SER |
| 13 | YB | 150[B] | SER |
| 13 | YB | 150[C] | SER |
| 13 | YB | 150[D] | SER |
| 13 | YB | 150[E] | SER |
| 13 | YB | 150[F] | SER |
| 13 | YB | 152[A] | LEU |
| 13 | YB | 152[B] | LEU |
| 13 | YB | 152[C] | LEU |
| 13 | YB | 152[D] | LEU |
| 13 | YB | 152[E] | LEU |
| 13 | YB | 152[F] | LEU |
| 13 | YB | 173[A] | ASN |
| 13 | YB | 173[B] | ASN |
| 13 | YB | 173[C] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 173[D] | ASN |
| 13 | YB | 173[E] | ASN |
| 13 | YB | 173[F] | ASN |
| 13 | YB | 180[A] | LEU |
| 13 | YB | 180[B] | LEU |
| 13 | YB | 180[C] | LEU |
| 13 | YB | 180[D] | LEU |
| 13 | YB | 180[E] | LEU |
| 13 | YB | 180[F] | LEU |
| 13 | YB | 182[A] | ARG |
| 13 | YB | 182[B] | ARG |
| 13 | YB | 182[C] | ARG |
| 13 | YB | 182[D] | ARG |
| 13 | YB | 182[E] | ARG |
| 13 | YB | 182[F] | ARG |
| 13 | YB | 195[A] | GLU |
| 13 | YB | 195[B] | GLU |
| 13 | YB | 195[C] | GLU |
| 13 | YB | 195[D] | GLU |
| 13 | YB | 195[E] | GLU |
| 13 | YB | 195[F] | GLU |
| 13 | YB | 209[A] | GLN |
| 13 | YB | 209[B] | GLN |
| 13 | YB | 209[C] | GLN |
| 13 | YB | 209[D] | GLN |
| 13 | YB | 209[E] | GLN |
| 13 | YB | 209[F] | GLN |
| 13 | YB | 242[A] | THR |
| 13 | YB | 242[B] | THR |
| 13 | YB | 242[C] | THR |
| 13 | YB | 242[D] | THR |
| 13 | YB | 242[E] | THR |
| 13 | YB | 242[F] | THR |
| 13 | YB | 296[A] | LEU |
| 13 | YB | 296[B] | LEU |
| 13 | YB | 296[C] | LEU |
| 13 | YB | 296[D] | LEU |
| 13 | YB | 296[E] | LEU |
| 13 | YB | 296[F] | LEU |
| 13 | YB | 300[A] | LEU |
| 13 | YB | 300[B] | LEU |
| 13 | YB | 300[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 300[D] | LEU |
| 13 | YB | 300[E] | LEU |
| 13 | YB | 300[F] | LEU |
| 13 | YB | 327[A] | VAL |
| 13 | YB | 327[B] | VAL |
| 13 | YB | 327[C] | VAL |
| 13 | YB | 327[D] | VAL |
| 13 | YB | 327[E] | VAL |
| 13 | YB | 327[F] | VAL |
| 13 | YB | 331[A] | ILE |
| 13 | YB | 331[B] | ILE |
| 13 | YB | 331[C] | ILE |
| 13 | YB | 331[D] | ILE |
| 13 | YB | 331[E] | ILE |
| 13 | YB | 331[F] | ILE |
| 13 | YB | 335[A] | ASN |
| 13 | YB | 335[B] | ASN |
| 13 | YB | 335[C] | ASN |
| 13 | YB | 335[D] | ASN |
| 13 | YB | 335[E] | ASN |
| 13 | YB | 335[F] | ASN |
| 13 | YB | 372[A] | SER |
| 13 | YB | 372[B] | SER |
| 13 | YB | 372[C] | SER |
| 13 | YB | 372[D] | SER |
| 13 | YB | 372[E] | SER |
| 13 | YB | 372[F] | SER |
| 13 | YB | 373[A] | ARG |
| 13 | YB | 373[B] | ARG |
| 13 | YB | 373[C] | ARG |
| 13 | YB | 373[D] | ARG |
| 13 | YB | 373[E] | ARG |
| 13 | YB | 373[F] | ARG |
| 13 | YB | 375[A] | LEU |
| 13 | YB | 375[B] | LEU |
| 13 | YB | 375[C] | LEU |
| 13 | YB | 375[D] | LEU |
| 13 | YB | 375[E] | LEU |
| 13 | YB | 375[F] | LEU |
| 13 | YB | 418[A] | THR |
| 13 | YB | 418[B] | THR |
| 13 | YB | 418[C] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 418[D] | THR |
| 13 | YB | 418[E] | THR |
| 13 | YB | 418[F] | THR |
| 13 | YB | 429[A] | ARG |
| 13 | YB | 429[B] | ARG |
| 13 | YB | 429[C] | ARG |
| 13 | YB | 429[D] | ARG |
| 13 | YB | 429[E] | ARG |
| 13 | YB | 429[F] | ARG |
| 13 | YB | 432[A] | ARG |
| 13 | YB | 432[B] | ARG |
| 13 | YB | 432[C] | ARG |
| 13 | YB | 432[D] | ARG |
| 13 | YB | 432[E] | ARG |
| 13 | YB | 432[F] | ARG |
| 13 | YB | 435[A] | VAL |
| 13 | YB | 435[B] | VAL |
| 13 | YB | 435[C] | VAL |
| 13 | YB | 435[D] | VAL |
| 13 | YB | 435[E] | VAL |
| 13 | YB | 435[F] | VAL |
| 13 | YB | 442[A] | THR |
| 13 | YB | 442[B] | THR |
| 13 | YB | 442[C] | THR |
| 13 | YB | 442[D] | THR |
| 13 | YB | 442[E] | THR |
| 13 | YB | 442[F] | THR |
| 13 | YB | 455[A] | LYS |
| 13 | YB | 455[B] | LYS |
| 13 | YB | 455[C] | LYS |
| 13 | YB | 455[D] | LYS |
| 13 | YB | 455[E] | LYS |
| 13 | YB | 455[F] | LYS |
| 13 | YB | 465[A] | TYR |
| 13 | YB | 465[B] | TYR |
| 13 | YB | 465[C] | TYR |
| 13 | YB | 465[D] | TYR |
| 13 | YB | 465[E] | TYR |
| 13 | YB | 465[F] | TYR |
| 13 | YB | 486[A] | GLU |
| 13 | YB | 486[B] | GLU |
| 13 | YB | 486[C] | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YB | 486[D] | GLU |
| 13 | YB | 486[E] | GLU |
| 13 | YB | 486[F] | GLU |
| 13 | YB | 522[A] | VAL |
| 13 | YB | 522[B] | VAL |
| 13 | YB | 522[C] | VAL |
| 13 | YB | 522[D] | VAL |
| 13 | YB | 522[E] | VAL |
| 13 | YB | 522[F] | VAL |
| 13 | YB | 550[A] | TRP |
| 13 | YB | 550[B] | TRP |
| 13 | YB | 550[C] | TRP |
| 13 | YB | 550[D] | TRP |
| 13 | YB | 550[E] | TRP |
| 13 | YB | 550[F] | TRP |
| 13 | YB | 554[A] | MET |
| 13 | YB | 554[B] | MET |
| 13 | YB | 554[C] | MET |
| 13 | YB | 554[D] | MET |
| 13 | YB | 554[E] | MET |
| 13 | YB | 554[F] | MET |
| 13 | YB | 566[A] | THR |
| 13 | YB | 566[B] | THR |
| 13 | YB | 566[C] | THR |
| 13 | YB | 566[D] | THR |
| 13 | YB | 566[E] | THR |
| 13 | YB | 566[F] | THR |
| 13 | YB | 573[A] | ASP |
| 13 | YB | 573[B] | ASP |
| 13 | YB | 573[C] | ASP |
| 13 | YB | 573[D] | ASP |
| 13 | YB | 573[E] | ASP |
| 13 | YB | 573[F] | ASP |
| 13 | YC | 7[A] | ASN |
| 13 | YC | 7[B] | ASN |
| 13 | YC | 7[C] | ASN |
| 13 | YC | 7[D] | ASN |
| 13 | YC | 7[E] | ASN |
| 13 | YC | 7[F] | ASN |
| 13 | YC | 24[A] | LEU |
| 13 | YC | 24[B] | LEU |
| 13 | YC | 24[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 24[D] | LEU |
| 13 | YC | 24[E] | LEU |
| 13 | YC | 24[F] | LEU |
| 13 | YC | 27[A] | VAL |
| 13 | YC | 27[B] | VAL |
| 13 | YC | 27[C] | VAL |
| 13 | YC | 27[D] | VAL |
| 13 | YC | 27[E] | VAL |
| 13 | YC | 27[F] | VAL |
| 13 | YC | 34[A] | LEU |
| 13 | YC | 34[B] | LEU |
| 13 | YC | 34[C] | LEU |
| 13 | YC | 34[D] | LEU |
| 13 | YC | 34[E] | LEU |
| 13 | YC | 34[F] | LEU |
| 13 | YC | 41[A] | GLN |
| 13 | YC | 41[B] | GLN |
| 13 | YC | 41[C] | GLN |
| 13 | YC | 41[D] | GLN |
| 13 | YC | 41[E] | GLN |
| 13 | YC | 41[F] | GLN |
| 13 | YC | 50[A] | GLU |
| 13 | YC | 50[B] | GLU |
| 13 | YC | 50[C] | GLU |
| 13 | YC | 50[D] | GLU |
| 13 | YC | 50[E] | GLU |
| 13 | YC | 50[F] | GLU |
| 13 | YC | 56[A] | SER |
| 13 | YC | 56[B] | SER |
| 13 | YC | 56[C] | SER |
| 13 | YC | 56[D] | SER |
| 13 | YC | 56[E] | SER |
| 13 | YC | 56[F] | SER |
| 13 | YC | 57[A] | VAL |
| 13 | YC | 57[B] | VAL |
| 13 | YC | 57[C] | VAL |
| 13 | YC | 57[D] | VAL |
| 13 | YC | 57[E] | VAL |
| 13 | YC | 57[F] | VAL |
| 13 | YC | 59[A] | GLN |
| 13 | YC | 59[B] | GLN |
| 13 | YC | 59[C] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 59[D] | GLN |
| 13 | YC | 59[E] | GLN |
| 13 | YC | 59[F] | GLN |
| 13 | YC | 61[A] | ILE |
| 13 | YC | 61[B] | ILE |
| 13 | YC | 61[C] | ILE |
| 13 | YC | 61[D] | ILE |
| 13 | YC | 61[E] | ILE |
| 13 | YC | 61[F] | ILE |
| 13 | YC | 66[A] | MET |
| 13 | YC | 66[B] | MET |
| 13 | YC | 66[C] | MET |
| 13 | YC | 66[D] | MET |
| 13 | YC | 66[E] | MET |
| 13 | YC | 66[F] | MET |
| 13 | YC | 82[A] | VAL |
| 13 | YC | 82[B] | VAL |
| 13 | YC | 82[C] | VAL |
| 13 | YC | 82[D] | VAL |
| 13 | YC | 82[E] | VAL |
| 13 | YC | 82[F] | VAL |
| 13 | YC | 87[A] | LEU |
| 13 | YC | 87[B] | LEU |
| 13 | YC | 87[C] | LEU |
| 13 | YC | 87[D] | LEU |
| 13 | YC | 87[E] | LEU |
| 13 | YC | 87[F] | LEU |
| 13 | YC | 89[A] | LYS |
| 13 | YC | 89[B] | LYS |
| 13 | YC | 89[C] | LYS |
| 13 | YC | 89[D] | LYS |
| 13 | YC | 89[E] | LYS |
| 13 | YC | 89[F] | LYS |
| 13 | YC | 97[A] | LEU |
| 13 | YC | 97[B] | LEU |
| 13 | YC | 97[C] | LEU |
| 13 | YC | 97[D] | LEU |
| 13 | YC | 97[E] | LEU |
| 13 | YC | 97[F] | LEU |
| 13 | YC | 127[A] | ASN |
| 13 | YC | 127[B] | ASN |
| 13 | YC | 127[C] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 127[D] | ASN |
| 13 | YC | 127[E] | ASN |
| 13 | YC | 127[F] | ASN |
| 13 | YC | 150[A] | SER |
| 13 | YC | 150[B] | SER |
| 13 | YC | 150[C] | SER |
| 13 | YC | 150[D] | SER |
| 13 | YC | 150[E] | SER |
| 13 | YC | 150[F] | SER |
| 13 | YC | 152[A] | LEU |
| 13 | YC | 152[B] | LEU |
| 13 | YC | 152[C] | LEU |
| 13 | YC | 152[D] | LEU |
| 13 | YC | 152[E] | LEU |
| 13 | YC | 152[F] | LEU |
| 13 | YC | 173[A] | ASN |
| 13 | YC | 173[B] | ASN |
| 13 | YC | 173[C] | ASN |
| 13 | YC | 173[D] | ASN |
| 13 | YC | 173[E] | ASN |
| 13 | YC | 173[F] | ASN |
| 13 | YC | 180[A] | LEU |
| 13 | YC | 180[B] | LEU |
| 13 | YC | 180[C] | LEU |
| 13 | YC | 180[D] | LEU |
| 13 | YC | 180[E] | LEU |
| 13 | YC | 180[F] | LEU |
| 13 | YC | 182[A] | ARG |
| 13 | YC | 182[B] | ARG |
| 13 | YC | 182[C] | ARG |
| 13 | YC | 182[D] | ARG |
| 13 | YC | 182[E] | ARG |
| 13 | YC | 182[F] | ARG |
| 13 | YC | 195[A] | GLU |
| 13 | YC | 195[B] | GLU |
| 13 | YC | 195[C] | GLU |
| 13 | YC | 195[D] | GLU |
| 13 | YC | 195[E] | GLU |
| 13 | YC | 195[F] | GLU |
| 13 | YC | 209[A] | GLN |
| 13 | YC | 209[B] | GLN |
| 13 | YC | 209[C] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 209[D] | GLN |
| 13 | YC | 209[E] | GLN |
| 13 | YC | 209[F] | GLN |
| 13 | YC | 242[A] | THR |
| 13 | YC | 242[B] | THR |
| 13 | YC | 242[C] | THR |
| 13 | YC | 242[D] | THR |
| 13 | YC | 242[E] | THR |
| 13 | YC | 242[F] | THR |
| 13 | YC | 296[A] | LEU |
| 13 | YC | 296[B] | LEU |
| 13 | YC | 296[C] | LEU |
| 13 | YC | 296[D] | LEU |
| 13 | YC | 296[E] | LEU |
| 13 | YC | 296[F] | LEU |
| 13 | YC | 300[A] | LEU |
| 13 | YC | 300[B] | LEU |
| 13 | YC | 300[C] | LEU |
| 13 | YC | 300[D] | LEU |
| 13 | YC | 300[E] | LEU |
| 13 | YC | 300[F] | LEU |
| 13 | YC | 327[A] | VAL |
| 13 | YC | 327[B] | VAL |
| 13 | YC | 327[C] | VAL |
| 13 | YC | 327[D] | VAL |
| 13 | YC | 327[E] | VAL |
| 13 | YC | 327[F] | VAL |
| 13 | YC | 331[A] | ILE |
| 13 | YC | 331[B] | ILE |
| 13 | YC | 331[C] | ILE |
| 13 | YC | 331[D] | ILE |
| 13 | YC | 331[E] | ILE |
| 13 | YC | 331[F] | ILE |
| 13 | YC | 335[A] | ASN |
| 13 | YC | 335[B] | ASN |
| 13 | YC | 335[C] | ASN |
| 13 | YC | 335[D] | ASN |
| 13 | YC | 335[E] | ASN |
| 13 | YC | 335[F] | ASN |
| 13 | YC | 372[A] | SER |
| 13 | YC | 372[B] | SER |
| 13 | YC | 372[C] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 372[D] | SER |
| 13 | YC | 372[E] | SER |
| 13 | YC | 372[F] | SER |
| 13 | YC | 373[A] | ARG |
| 13 | YC | 373[B] | ARG |
| 13 | YC | 373[C] | ARG |
| 13 | YC | 373[D] | ARG |
| 13 | YC | 373[E] | ARG |
| 13 | YC | 373[F] | ARG |
| 13 | YC | 375[A] | LEU |
| 13 | YC | 375[B] | LEU |
| 13 | YC | 375[C] | LEU |
| 13 | YC | 375[D] | LEU |
| 13 | YC | 375[E] | LEU |
| 13 | YC | 375[F] | LEU |
| 13 | YC | 418[A] | THR |
| 13 | YC | 418[B] | THR |
| 13 | YC | 418[C] | THR |
| 13 | YC | 418[D] | THR |
| 13 | YC | 418[E] | THR |
| 13 | YC | 418[F] | THR |
| 13 | YC | 429[A] | ARG |
| 13 | YC | 429[B] | ARG |
| 13 | YC | 429[C] | ARG |
| 13 | YC | 429[D] | ARG |
| 13 | YC | 429[E] | ARG |
| 13 | YC | 429[F] | ARG |
| 13 | YC | 432[A] | ARG |
| 13 | YC | 432[B] | ARG |
| 13 | YC | 432[C] | ARG |
| 13 | YC | 432[D] | ARG |
| 13 | YC | 432[E] | ARG |
| 13 | YC | 432[F] | ARG |
| 13 | YC | 435[A] | VAL |
| 13 | YC | 435[B] | VAL |
| 13 | YC | 435[C] | VAL |
| 13 | YC | 435[D] | VAL |
| 13 | YC | 435[E] | VAL |
| 13 | YC | 435[F] | VAL |
| 13 | YC | 442[A] | THR |
| 13 | YC | 442[B] | THR |
| 13 | YC | 442[C] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 442[D] | THR |
| 13 | YC | 442[E] | THR |
| 13 | YC | 442[F] | THR |
| 13 | YC | 455[A] | LYS |
| 13 | YC | 455[B] | LYS |
| 13 | YC | 455[C] | LYS |
| 13 | YC | 455[D] | LYS |
| 13 | YC | 455[E] | LYS |
| 13 | YC | 455[F] | LYS |
| 13 | YC | 465[A] | TYR |
| 13 | YC | 465[B] | TYR |
| 13 | YC | 465[C] | TYR |
| 13 | YC | 465[D] | TYR |
| 13 | YC | 465[E] | TYR |
| 13 | YC | 465[F] | TYR |
| 13 | YC | 486[A] | GLU |
| 13 | YC | 486[B] | GLU |
| 13 | YC | 486[C] | GLU |
| 13 | YC | 486[D] | GLU |
| 13 | YC | 486[E] | GLU |
| 13 | YC | 486[F] | GLU |
| 13 | YC | 522[A] | VAL |
| 13 | YC | 522[B] | VAL |
| 13 | YC | 522[C] | VAL |
| 13 | YC | 522[D] | VAL |
| 13 | YC | 522[E] | VAL |
| 13 | YC | 522[F] | VAL |
| 13 | YC | 550[A] | TRP |
| 13 | YC | 550[B] | TRP |
| 13 | YC | 550[C] | TRP |
| 13 | YC | 550[D] | TRP |
| 13 | YC | 550[E] | TRP |
| 13 | YC | 550[F] | TRP |
| 13 | YC | 554[A] | MET |
| 13 | YC | 554[B] | MET |
| 13 | YC | 554[C] | MET |
| 13 | YC | 554[D] | MET |
| 13 | YC | 554[E] | MET |
| 13 | YC | 554[F] | MET |
| 13 | YC | 566[A] | THR |
| 13 | YC | 566[B] | THR |
| 13 | YC | 566[C] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | YC | 566[D] | THR |
| 13 | YC | 566[E] | THR |
| 13 | YC | 566[F] | THR |
| 13 | YC | 573[A] | ASP |
| 13 | YC | 573[B] | ASP |
| 13 | YC | 573[C] | ASP |
| 13 | YC | 573[D] | ASP |
| 13 | YC | 573[E] | ASP |
| 13 | YC | 573[F] | ASP |
| 14 | YD | 15[A] | LYS |
| 14 | YD | 15[B] | LYS |
| 14 | YD | 15[C] | LYS |
| 14 | YD | 15[D] | LYS |
| 14 | YD | 15[E] | LYS |
| 14 | YD | 15[F] | LYS |
| 14 | YD | 16[A] | LEU |
| 14 | YD | 16[B] | LEU |
| 14 | YD | 16[C] | LEU |
| 14 | YD | 16[D] | LEU |
| 14 | YD | 16[E] | LEU |
| 14 | YD | 16[F] | LEU |
| 14 | YD | 21[A] | ASP |
| 14 | YD | 21[B] | ASP |
| 14 | YD | 21[C] | ASP |
| 14 | YD | 21[D] | ASP |
| 14 | YD | 21[E] | ASP |
| 14 | YD | 21[F] | ASP |
| 14 | YD | 35[A] | ILE |
| 14 | YD | 35[B] | ILE |
| 14 | YD | 35[C] | ILE |
| 14 | YD | 35[D] | ILE |
| 14 | YD | 35[E] | ILE |
| 14 | YD | 35[F] | ILE |
| 14 | YD | 42[A] | ASP |
| 14 | YD | 42[B] | ASP |
| 14 | YD | 42[C] | ASP |
| 14 | YD | 42[D] | ASP |
| 14 | YD | 42[E] | ASP |
| 14 | YD | 42[F] | ASP |
| 14 | YD | 44[A] | LEU |
| 14 | YD | 44[B] | LEU |
| 14 | YD | 44[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YD | 44[D] | LEU |
| 14 | YD | 44[E] | LEU |
| 14 | YD | 44[F] | LEU |
| 14 | YD | 51[A] | MET |
| 14 | YD | 51[B] | MET |
| 14 | YD | 51[C] | MET |
| 14 | YD | 51[D] | MET |
| 14 | YD | 51[E] | MET |
| 14 | YD | 51[F] | MET |
| 14 | YD | 58[A] | LYS |
| 14 | YD | 58[B] | LYS |
| 14 | YD | 58[C] | LYS |
| 14 | YD | 58[D] | LYS |
| 14 | YD | 58[E] | LYS |
| 14 | YD | 58[F] | LYS |
| 14 | YD | 68[A] | GLU |
| 14 | YD | 68[B] | GLU |
| 14 | YD | 68[C] | GLU |
| 14 | YD | 68[D] | GLU |
| 14 | YD | 68[E] | GLU |
| 14 | YD | 68[F] | GLU |
| 14 | YD | 74[A] | VAL |
| 14 | YD | 74[B] | VAL |
| 14 | YD | 74[C] | VAL |
| 14 | YD | 74[D] | VAL |
| 14 | YD | 74[E] | VAL |
| 14 | YD | 74[F] | VAL |
| 14 | YD | 80[A] | ILE |
| 14 | YD | 80[B] | ILE |
| 14 | YD | 80[C] | ILE |
| 14 | YD | 80[D] | ILE |
| 14 | YD | 80[E] | ILE |
| 14 | YD | 80[F] | ILE |
| 14 | YD | 87[A] | ILE |
| 14 | YD | 87[B] | ILE |
| 14 | YD | 87[C] | ILE |
| 14 | YD | 87[D] | ILE |
| 14 | YD | 87[E] | ILE |
| 14 | YD | 87[F] | ILE |
| 14 | YD | 90[A] | CYS |
| 14 | YD | 90[B] | CYS |
| 14 | YD | 90[C] | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YD | 90[D] | CYS |
| 14 | YD | 90[E] | CYS |
| 14 | YD | 90[F] | CYS |
| 14 | YD | 104[A] | ILE |
| 14 | YD | 104[B] | ILE |
| 14 | YD | 104[C] | ILE |
| 14 | YD | 104[D] | ILE |
| 14 | YD | 104[E] | ILE |
| 14 | YD | 104[F] | ILE |
| 14 | YD | 107[A] | ILE |
| 14 | YD | 107[B] | ILE |
| 14 | YD | 107[C] | ILE |
| 14 | YD | 107[D] | ILE |
| 14 | YD | 107[E] | ILE |
| 14 | YD | 107[F] | ILE |
| 14 | YD | 109[A] | LEU |
| 14 | YD | 109[B] | LEU |
| 14 | YD | 109[C] | LEU |
| 14 | YD | 109[D] | LEU |
| 14 | YD | 109[E] | LEU |
| 14 | YD | 109[F] | LEU |
| 14 | YD | 111[A] | THR |
| 14 | YD | 111[B] | THR |
| 14 | YD | 111[C] | THR |
| 14 | YD | 111[D] | THR |
| 14 | YD | 111[E] | THR |
| 14 | YD | 111[F] | THR |
| 14 | YD | 154[A] | ASN |
| 14 | YD | 154[B] | ASN |
| 14 | YD | 154[C] | ASN |
| 14 | YD | 154[D] | ASN |
| 14 | YD | 154[E] | ASN |
| 14 | YD | 154[F] | ASN |
| 14 | YD | 163[A] | THR |
| 14 | YD | 163[B] | THR |
| 14 | YD | 163[C] | THR |
| 14 | YD | 163[D] | THR |
| 14 | YD | 163[E] | THR |
| 14 | YD | 163[F] | THR |
| 14 | YD | 183[A] | ASP |
| 14 | YD | 183[B] | ASP |
| 14 | YD | 183[C] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YD | 183[D] | ASP |
| 14 | YD | 183[E] | ASP |
| 14 | YD | 183[F] | ASP |
| 14 | YD | 233[A] | ASP |
| 14 | YD | 233[B] | ASP |
| 14 | YD | 233[C] | ASP |
| 14 | YD | 233[D] | ASP |
| 14 | YD | 233[E] | ASP |
| 14 | YD | 233[F] | ASP |
| 14 | YD | 236[A] | TRP |
| 14 | YD | 236[B] | TRP |
| 14 | YD | 236[C] | TRP |
| 14 | YD | 236[D] | TRP |
| 14 | YD | 236[E] | TRP |
| 14 | YD | 236[F] | TRP |
| 14 | YD | 241[A] | ASN |
| 14 | YD | 241[B] | ASN |
| 14 | YD | 241[C] | ASN |
| 14 | YD | 241[D] | ASN |
| 14 | YD | 241[E] | ASN |
| 14 | YD | 241[F] | ASN |
| 14 | YD | 267[A] | THR |
| 14 | YD | 267[B] | THR |
| 14 | YD | 267[C] | THR |
| 14 | YD | 267[D] | THR |
| 14 | YD | 267[E] | THR |
| 14 | YD | 267[F] | THR |
| 14 | YD | 296[A] | ILE |
| 14 | YD | 296[B] | ILE |
| 14 | YD | 296[C] | ILE |
| 14 | YD | 296[D] | ILE |
| 14 | YD | 296[E] | ILE |
| 14 | YD | 296[F] | ILE |
| 14 | YD | 305[A] | ASP |
| 14 | YD | 305[B] | ASP |
| 14 | YD | 305[C] | ASP |
| 14 | YD | 305[D] | ASP |
| 14 | YD | 305[E] | ASP |
| 14 | YD | 305[F] | ASP |
| 14 | YD | 312[A] | THR |
| 14 | YD | 312[B] | THR |
| 14 | YD | 312[C] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YD | 312[D] | THR |
| 14 | YD | 312[E] | THR |
| 14 | YD | 312[F] | THR |
| 14 | YD | 315[A] | ASN |
| 14 | YD | 315[B] | ASN |
| 14 | YD | 315[C] | ASN |
| 14 | YD | 315[D] | ASN |
| 14 | YD | 315[E] | ASN |
| 14 | YD | 315[F] | ASN |
| 14 | YD | 318[A] | LEU |
| 14 | YD | 318[B] | LEU |
| 14 | YD | 318[C] | LEU |
| 14 | YD | 318[D] | LEU |
| 14 | YD | 318[E] | LEU |
| 14 | YD | 318[F] | LEU |
| 14 | YD | 325[A] | ILE |
| 14 | YD | 325[B] | ILE |
| 14 | YD | 325[C] | ILE |
| 14 | YD | 325[D] | ILE |
| 14 | YD | 325[E] | ILE |
| 14 | YD | 325[F] | ILE |
| 14 | YD | 330[A] | LYS |
| 14 | YD | 330[B] | LYS |
| 14 | YD | 330[C] | LYS |
| 14 | YD | 330[D] | LYS |
| 14 | YD | 330[E] | LYS |
| 14 | YD | 330[F] | LYS |
| 14 | YD | 333[A] | PHE |
| 14 | YD | 333[B] | PHE |
| 14 | YD | 333[C] | PHE |
| 14 | YD | 333[D] | PHE |
| 14 | YD | 333[E] | PHE |
| 14 | YD | 333[F] | PHE |
| 14 | YD | 342[A] | VAL |
| 14 | YD | 342[B] | VAL |
| 14 | YD | 342[C] | VAL |
| 14 | YD | 342[D] | VAL |
| 14 | YD | 342[E] | VAL |
| 14 | YD | 342[F] | VAL |
| 14 | YD | 346[A] | LEU |
| 14 | YD | 346[B] | LEU |
| 14 | YD | 346[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YD | 346[D] | LEU |
| 14 | YD | 346[E] | LEU |
| 14 | YD | 346[F] | LEU |
| 14 | YD | 352[A] | VAL |
| 14 | YD | 352[B] | VAL |
| 14 | YD | 352[C] | VAL |
| 14 | YD | 352[D] | VAL |
| 14 | YD | 352[E] | VAL |
| 14 | YD | 352[F] | VAL |
| 14 | YD | 360[A] | ASN |
| 14 | YD | 360[B] | ASN |
| 14 | YD | 360[C] | ASN |
| 14 | YD | 360[D] | ASN |
| 14 | YD | 360[E] | ASN |
| 14 | YD | 360[F] | ASN |
| 14 | YD | 364[A] | LEU |
| 14 | YD | 364[B] | LEU |
| 14 | YD | 364[C] | LEU |
| 14 | YD | 364[D] | LEU |
| 14 | YD | 364[E] | LEU |
| 14 | YD | 364[F] | LEU |
| 14 | YD | 365[A] | GLU |
| 14 | YD | 365[B] | GLU |
| 14 | YD | 365[C] | GLU |
| 14 | YD | 365[D] | GLU |
| 14 | YD | 365[E] | GLU |
| 14 | YD | 365[F] | GLU |
| 14 | YD | 366[A] | THR |
| 14 | YD | 366[B] | THR |
| 14 | YD | 366[C] | THR |
| 14 | YD | 366[D] | THR |
| 14 | YD | 366[E] | THR |
| 14 | YD | 366[F] | THR |
| 14 | YE | 15[A] | LYS |
| 14 | YE | 15[B] | LYS |
| 14 | YE | 15[C] | LYS |
| 14 | YE | 15[D] | LYS |
| 14 | YE | 15[E] | LYS |
| 14 | YE | 15[F] | LYS |
| 14 | YE | 16[A] | LEU |
| 14 | YE | 16[B] | LEU |
| 14 | YE | 16[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 16[D] | LEU |
| 14 | YE | 16[E] | LEU |
| 14 | YE | 16[F] | LEU |
| 14 | YE | 21[A] | ASP |
| 14 | YE | 21[B] | ASP |
| 14 | YE | 21[C] | ASP |
| 14 | YE | 21[D] | ASP |
| 14 | YE | 21[E] | ASP |
| 14 | YE | 21[F] | ASP |
| 14 | YE | 35[A] | ILE |
| 14 | YE | 35[B] | ILE |
| 14 | YE | 35[C] | ILE |
| 14 | YE | 35[D] | ILE |
| 14 | YE | 35[E] | ILE |
| 14 | YE | 35[F] | ILE |
| 14 | YE | 42[A] | ASP |
| 14 | YE | 42[B] | ASP |
| 14 | YE | 42[C] | ASP |
| 14 | YE | 42[D] | ASP |
| 14 | YE | 42[E] | ASP |
| 14 | YE | 42[F] | ASP |
| 14 | YE | 44[A] | LEU |
| 14 | YE | 44[B] | LEU |
| 14 | YE | 44[C] | LEU |
| 14 | YE | 44[D] | LEU |
| 14 | YE | 44[E] | LEU |
| 14 | YE | 44[F] | LEU |
| 14 | YE | 51[A] | MET |
| 14 | YE | 51[B] | MET |
| 14 | YE | 51[C] | MET |
| 14 | YE | 51[D] | MET |
| 14 | YE | 51[E] | MET |
| 14 | YE | 51[F] | MET |
| 14 | YE | 58[A] | LYS |
| 14 | YE | 58[B] | LYS |
| 14 | YE | 58[C] | LYS |
| 14 | YE | 58[D] | LYS |
| 14 | YE | 58[E] | LYS |
| 14 | YE | 58[F] | LYS |
| 14 | YE | 68[A] | GLU |
| 14 | YE | 68[B] | GLU |
| 14 | YE | 68[C] | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 68[D] | GLU |
| 14 | YE | 68[E] | GLU |
| 14 | YE | 68[F] | GLU |
| 14 | YE | 74[A] | VAL |
| 14 | YE | 74[B] | VAL |
| 14 | YE | 74[C] | VAL |
| 14 | YE | 74[D] | VAL |
| 14 | YE | 74[E] | VAL |
| 14 | YE | 74[F] | VAL |
| 14 | YE | 80[A] | ILE |
| 14 | YE | 80[B] | ILE |
| 14 | YE | 80[C] | ILE |
| 14 | YE | 80[D] | ILE |
| 14 | YE | 80[E] | ILE |
| 14 | YE | 80[F] | ILE |
| 14 | YE | 87[A] | ILE |
| 14 | YE | 87[B] | ILE |
| 14 | YE | 87[C] | ILE |
| 14 | YE | 87[D] | ILE |
| 14 | YE | 87[E] | ILE |
| 14 | YE | 87[F] | ILE |
| 14 | YE | 90[A] | CYS |
| 14 | YE | 90[B] | CYS |
| 14 | YE | 90[C] | CYS |
| 14 | YE | 90[D] | CYS |
| 14 | YE | 90[E] | CYS |
| 14 | YE | 90[F] | CYS |
| 14 | YE | 104[A] | ILE |
| 14 | YE | 104[B] | ILE |
| 14 | YE | 104[C] | ILE |
| 14 | YE | 104[D] | ILE |
| 14 | YE | 104[E] | ILE |
| 14 | YE | 104[F] | ILE |
| 14 | YE | 107[A] | ILE |
| 14 | YE | 107[B] | ILE |
| 14 | YE | 107[C] | ILE |
| 14 | YE | 107[D] | ILE |
| 14 | YE | 107[E] | ILE |
| 14 | YE | 107[F] | ILE |
| 14 | YE | 109[A] | LEU |
| 14 | YE | 109[B] | LEU |
| 14 | YE | 109[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 109[D] | LEU |
| 14 | YE | 109[E] | LEU |
| 14 | YE | 109[F] | LEU |
| 14 | YE | 111[A] | THR |
| 14 | YE | 111[B] | THR |
| 14 | YE | 111[C] | THR |
| 14 | YE | 111[D] | THR |
| 14 | YE | 111[E] | THR |
| 14 | YE | 111[F] | THR |
| 14 | YE | 154[A] | ASN |
| 14 | YE | 154[B] | ASN |
| 14 | YE | 154[C] | ASN |
| 14 | YE | 154[D] | ASN |
| 14 | YE | 154[E] | ASN |
| 14 | YE | 154[F] | ASN |
| 14 | YE | 163[A] | THR |
| 14 | YE | 163[B] | THR |
| 14 | YE | 163[C] | THR |
| 14 | YE | 163[D] | THR |
| 14 | YE | 163[E] | THR |
| 14 | YE | 163[F] | THR |
| 14 | YE | 183[A] | ASP |
| 14 | YE | 183[B] | ASP |
| 14 | YE | 183[C] | ASP |
| 14 | YE | 183[D] | ASP |
| 14 | YE | 183[E] | ASP |
| 14 | YE | 183[F] | ASP |
| 14 | YE | 233[A] | ASP |
| 14 | YE | 233[B] | ASP |
| 14 | YE | 233[C] | ASP |
| 14 | YE | 233[D] | ASP |
| 14 | YE | 233[E] | ASP |
| 14 | YE | 233[F] | ASP |
| 14 | YE | 236[A] | TRP |
| 14 | YE | 236[B] | TRP |
| 14 | YE | 236[C] | TRP |
| 14 | YE | 236[D] | TRP |
| 14 | YE | 236[E] | TRP |
| 14 | YE | 236[F] | TRP |
| 14 | YE | 241[A] | ASN |
| 14 | YE | 241[B] | ASN |
| 14 | YE | 241[C] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 241[D] | ASN |
| 14 | YE | 241[E] | ASN |
| 14 | YE | 241[F] | ASN |
| 14 | YE | 267[A] | THR |
| 14 | YE | 267[B] | THR |
| 14 | YE | 267[C] | THR |
| 14 | YE | 267[D] | THR |
| 14 | YE | 267[E] | THR |
| 14 | YE | 267[F] | THR |
| 14 | YE | 296[A] | ILE |
| 14 | YE | 296[B] | ILE |
| 14 | YE | 296[C] | ILE |
| 14 | YE | 296[D] | ILE |
| 14 | YE | 296[E] | ILE |
| 14 | YE | 296[F] | ILE |
| 14 | YE | 305[A] | ASP |
| 14 | YE | 305[B] | ASP |
| 14 | YE | 305[C] | ASP |
| 14 | YE | 305[D] | ASP |
| 14 | YE | 305[E] | ASP |
| 14 | YE | 305[F] | ASP |
| 14 | YE | 312[A] | THR |
| 14 | YE | 312[B] | THR |
| 14 | YE | 312[C] | THR |
| 14 | YE | 312[D] | THR |
| 14 | YE | 312[E] | THR |
| 14 | YE | 312[F] | THR |
| 14 | YE | 315[A] | ASN |
| 14 | YE | 315[B] | ASN |
| 14 | YE | 315[C] | ASN |
| 14 | YE | 315[D] | ASN |
| 14 | YE | 315[E] | ASN |
| 14 | YE | 315[F] | ASN |
| 14 | YE | 318[A] | LEU |
| 14 | YE | 318[B] | LEU |
| 14 | YE | 318[C] | LEU |
| 14 | YE | 318[D] | LEU |
| 14 | YE | 318[E] | LEU |
| 14 | YE | 318[F] | LEU |
| 14 | YE | 325[A] | ILE |
| 14 | YE | 325[B] | ILE |
| 14 | YE | 325[C] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 325[D] | ILE |
| 14 | YE | 325[E] | ILE |
| 14 | YE | 325[F] | ILE |
| 14 | YE | 330[A] | LYS |
| 14 | YE | 330[B] | LYS |
| 14 | YE | 330[C] | LYS |
| 14 | YE | 330[D] | LYS |
| 14 | YE | 330[E] | LYS |
| 14 | YE | 330[F] | LYS |
| 14 | YE | 333[A] | PHE |
| 14 | YE | 333[B] | PHE |
| 14 | YE | 333[C] | PHE |
| 14 | YE | 333[D] | PHE |
| 14 | YE | 333[E] | PHE |
| 14 | YE | 333[F] | PHE |
| 14 | YE | 342[A] | VAL |
| 14 | YE | 342[B] | VAL |
| 14 | YE | 342[C] | VAL |
| 14 | YE | 342[D] | VAL |
| 14 | YE | 342[E] | VAL |
| 14 | YE | 342[F] | VAL |
| 14 | YE | 346[A] | LEU |
| 14 | YE | 346[B] | LEU |
| 14 | YE | 346[C] | LEU |
| 14 | YE | 346[D] | LEU |
| 14 | YE | 346[E] | LEU |
| 14 | YE | 346[F] | LEU |
| 14 | YE | 352[A] | VAL |
| 14 | YE | 352[B] | VAL |
| 14 | YE | 352[C] | VAL |
| 14 | YE | 352[D] | VAL |
| 14 | YE | 352[E] | VAL |
| 14 | YE | 352[F] | VAL |
| 14 | YE | 360[A] | ASN |
| 14 | YE | 360[B] | ASN |
| 14 | YE | 360[C] | ASN |
| 14 | YE | 360[D] | ASN |
| 14 | YE | 360[E] | ASN |
| 14 | YE | 360[F] | ASN |
| 14 | YE | 364[A] | LEU |
| 14 | YE | 364[B] | LEU |
| 14 | YE | 364[C] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YE | 364[D] | LEU |
| 14 | YE | 364[E] | LEU |
| 14 | YE | 364[F] | LEU |
| 14 | YE | 365[A] | GLU |
| 14 | YE | 365[B] | GLU |
| 14 | YE | 365[C] | GLU |
| 14 | YE | 365[D] | GLU |
| 14 | YE | 365[E] | GLU |
| 14 | YE | 365[F] | GLU |
| 14 | YE | 366[A] | THR |
| 14 | YE | 366[B] | THR |
| 14 | YE | 366[C] | THR |
| 14 | YE | 366[D] | THR |
| 14 | YE | 366[E] | THR |
| 14 | YE | 366[F] | THR |
| 14 | YF | 15[A] | LYS |
| 14 | YF | 15[B] | LYS |
| 14 | YF | 15[C] | LYS |
| 14 | YF | 15[D] | LYS |
| 14 | YF | 15[E] | LYS |
| 14 | YF | 15[F] | LYS |
| 14 | YF | 16[A] | LEU |
| 14 | YF | 16[B] | LEU |
| 14 | YF | 16[C] | LEU |
| 14 | YF | 16[D] | LEU |
| 14 | YF | 16[E] | LEU |
| 14 | YF | 16[F] | LEU |
| 14 | YF | 21[A] | ASP |
| 14 | YF | 21[B] | ASP |
| 14 | YF | 21[C] | ASP |
| 14 | YF | 21[D] | ASP |
| 14 | YF | 21[E] | ASP |
| 14 | YF | 21[F] | ASP |
| 14 | YF | 35[A] | ILE |
| 14 | YF | 35[B] | ILE |
| 14 | YF | 35[C] | ILE |
| 14 | YF | 35[D] | ILE |
| 14 | YF | 35[E] | ILE |
| 14 | YF | 35[F] | ILE |
| 14 | YF | 42[A] | ASP |
| 14 | YF | 42[B] | ASP |
| 14 | YF | 42[C] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YF | 42[D] | ASP |
| 14 | YF | 42[E] | ASP |
| 14 | YF | 42[F] | ASP |
| 14 | YF | 44[A] | LEU |
| 14 | YF | 44[B] | LEU |
| 14 | YF | 44[C] | LEU |
| 14 | YF | 44[D] | LEU |
| 14 | YF | 44[E] | LEU |
| 14 | YF | 44[F] | LEU |
| 14 | YF | 51[A] | MET |
| 14 | YF | 51[B] | MET |
| 14 | YF | 51[C] | MET |
| 14 | YF | 51[D] | MET |
| 14 | YF | 51[E] | MET |
| 14 | YF | 51[F] | MET |
| 14 | YF | 58[A] | LYS |
| 14 | YF | 58[B] | LYS |
| 14 | YF | 58[C] | LYS |
| 14 | YF | 58[D] | LYS |
| 14 | YF | 58[E] | LYS |
| 14 | YF | 58[F] | LYS |
| 14 | YF | 68[A] | GLU |
| 14 | YF | 68[B] | GLU |
| 14 | YF | 68[C] | GLU |
| 14 | YF | 68[D] | GLU |
| 14 | YF | 68[E] | GLU |
| 14 | YF | 68[F] | GLU |
| 14 | YF | 74[A] | VAL |
| 14 | YF | 74[B] | VAL |
| 14 | YF | 74[C] | VAL |
| 14 | YF | 74[D] | VAL |
| 14 | YF | 74[E] | VAL |
| 14 | YF | 74[F] | VAL |
| 14 | YF | 80[A] | ILE |
| 14 | YF | 80[B] | ILE |
| 14 | YF | 80[C] | ILE |
| 14 | YF | 80[D] | ILE |
| 14 | YF | 80[E] | ILE |
| 14 | YF | 80[F] | ILE |
| 14 | YF | 87[A] | ILE |
| 14 | YF | 87[B] | ILE |
| 14 | YF | 87[C] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YF | 87[D] | ILE |
| 14 | YF | 87[E] | ILE |
| 14 | YF | 87[F] | ILE |
| 14 | YF | 90[A] | CYS |
| 14 | YF | 90[B] | CYS |
| 14 | YF | 90[C] | CYS |
| 14 | YF | 90[D] | CYS |
| 14 | YF | 90[E] | CYS |
| 14 | YF | 90[F] | CYS |
| 14 | YF | 104[A] | ILE |
| 14 | YF | 104[B] | ILE |
| 14 | YF | 104[C] | ILE |
| 14 | YF | 104[D] | ILE |
| 14 | YF | 104[E] | ILE |
| 14 | YF | 104[F] | ILE |
| 14 | YF | 107[A] | ILE |
| 14 | YF | 107[B] | ILE |
| 14 | YF | 107[C] | ILE |
| 14 | YF | 107[D] | ILE |
| 14 | YF | 107[E] | ILE |
| 14 | YF | 107[F] | ILE |
| 14 | YF | 109[A] | LEU |
| 14 | YF | 109[B] | LEU |
| 14 | YF | 109[C] | LEU |
| 14 | YF | 109[D] | LEU |
| 14 | YF | 109[E] | LEU |
| 14 | YF | 109[F] | LEU |
| 14 | YF | 111[A] | THR |
| 14 | YF | 111[B] | THR |
| 14 | YF | 111[C] | THR |
| 14 | YF | 111[D] | THR |
| 14 | YF | 111[E] | THR |
| 14 | YF | 111[F] | THR |
| 14 | YF | 154[A] | ASN |
| 14 | YF | 154[B] | ASN |
| 14 | YF | 154[C] | ASN |
| 14 | YF | 154[D] | ASN |
| 14 | YF | 154[E] | ASN |
| 14 | YF | 154[F] | ASN |
| 14 | YF | 163[A] | THR |
| 14 | YF | 163[B] | THR |
| 14 | YF | 163[C] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YF | 163[D] | THR |
| 14 | YF | 163[E] | THR |
| 14 | YF | 163[F] | THR |
| 14 | YF | 183[A] | ASP |
| 14 | YF | 183[B] | ASP |
| 14 | YF | 183[C] | ASP |
| 14 | YF | 183[D] | ASP |
| 14 | YF | 183[E] | ASP |
| 14 | YF | 183[F] | ASP |
| 14 | YF | 233[A] | ASP |
| 14 | YF | 233[B] | ASP |
| 14 | YF | 233[C] | ASP |
| 14 | YF | 233[D] | ASP |
| 14 | YF | 233[E] | ASP |
| 14 | YF | 233[F] | ASP |
| 14 | YF | 236[A] | TRP |
| 14 | YF | 236[B] | TRP |
| 14 | YF | 236[C] | TRP |
| 14 | YF | 236[D] | TRP |
| 14 | YF | 236[E] | TRP |
| 14 | YF | 236[F] | TRP |
| 14 | YF | 241[A] | ASN |
| 14 | YF | 241[B] | ASN |
| 14 | YF | 241[C] | ASN |
| 14 | YF | 241[D] | ASN |
| 14 | YF | 241[E] | ASN |
| 14 | YF | 241[F] | ASN |
| 14 | YF | 267[A] | THR |
| 14 | YF | 267[B] | THR |
| 14 | YF | 267[C] | THR |
| 14 | YF | 267[D] | THR |
| 14 | YF | 267[E] | THR |
| 14 | YF | 267[F] | THR |
| 14 | YF | 296[A] | ILE |
| 14 | YF | 296[B] | ILE |
| 14 | YF | 296[C] | ILE |
| 14 | YF | 296[D] | ILE |
| 14 | YF | 296[E] | ILE |
| 14 | YF | 296[F] | ILE |
| 14 | YF | 305[A] | ASP |
| 14 | YF | 305[B] | ASP |
| 14 | YF | 305[C] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YF | 305[D] | ASP |
| 14 | YF | 305[E] | ASP |
| 14 | YF | 305[F] | ASP |
| 14 | YF | 312[A] | THR |
| 14 | YF | 312[B] | THR |
| 14 | YF | 312[C] | THR |
| 14 | YF | 312[D] | THR |
| 14 | YF | 312[E] | THR |
| 14 | YF | 312[F] | THR |
| 14 | YF | 315[A] | ASN |
| 14 | YF | 315[B] | ASN |
| 14 | YF | 315[C] | ASN |
| 14 | YF | 315[D] | ASN |
| 14 | YF | 315[E] | ASN |
| 14 | YF | 315[F] | ASN |
| 14 | YF | 318[A] | LEU |
| 14 | YF | 318[B] | LEU |
| 14 | YF | 318[C] | LEU |
| 14 | YF | 318[D] | LEU |
| 14 | YF | 318[E] | LEU |
| 14 | YF | 318[F] | LEU |
| 14 | YF | 325[A] | ILE |
| 14 | YF | 325[B] | ILE |
| 14 | YF | 325[C] | ILE |
| 14 | YF | 325[D] | ILE |
| 14 | YF | 325[E] | ILE |
| 14 | YF | 325[F] | ILE |
| 14 | YF | 330[A] | LYS |
| 14 | YF | 330[B] | LYS |
| 14 | YF | 330[C] | LYS |
| 14 | YF | 330[D] | LYS |
| 14 | YF | 330[E] | LYS |
| 14 | YF | 330[F] | LYS |
| 14 | YF | 333[A] | PHE |
| 14 | YF | 333[B] | PHE |
| 14 | YF | 333[C] | PHE |
| 14 | YF | 333[D] | PHE |
| 14 | YF | 333[E] | PHE |
| 14 | YF | 333[F] | PHE |
| 14 | YF | 342[A] | VAL |
| 14 | YF | 342[B] | VAL |
| 14 | YF | 342[C] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | YF | 342[D] | VAL |
| 14 | YF | 342[E] | VAL |
| 14 | YF | 342[F] | VAL |
| 14 | YF | 346[A] | LEU |
| 14 | YF | 346[B] | LEU |
| 14 | YF | 346[C] | LEU |
| 14 | YF | 346[D] | LEU |
| 14 | YF | 346[E] | LEU |
| 14 | YF | 346[F] | LEU |
| 14 | YF | 352[A] | VAL |
| 14 | YF | 352[B] | VAL |
| 14 | YF | 352[C] | VAL |
| 14 | YF | 352[D] | VAL |
| 14 | YF | 352[E] | VAL |
| 14 | YF | 352[F] | VAL |
| 14 | YF | 360[A] | ASN |
| 14 | YF | 360[B] | ASN |
| 14 | YF | 360[C] | ASN |
| 14 | YF | 360[D] | ASN |
| 14 | YF | 360[E] | ASN |
| 14 | YF | 360[F] | ASN |
| 14 | YF | 364[A] | LEU |
| 14 | YF | 364[B] | LEU |
| 14 | YF | 364[C] | LEU |
| 14 | YF | 364[D] | LEU |
| 14 | YF | 364[E] | LEU |
| 14 | YF | 364[F] | LEU |
| 14 | YF | 365[A] | GLU |
| 14 | YF | 365[B] | GLU |
| 14 | YF | 365[C] | GLU |
| 14 | YF | 365[D] | GLU |
| 14 | YF | 365[E] | GLU |
| 14 | YF | 365[F] | GLU |
| 14 | YF | 366[A] | THR |
| 14 | YF | 366[B] | THR |
| 14 | YF | 366[C] | THR |
| 14 | YF | 366[D] | THR |
| 14 | YF | 366[E] | THR |
| 14 | YF | 366[F] | THR |
| 15 | ZA | 26[A] | GLN |
| 15 | ZA | 26[B] | GLN |
| 15 | ZA | 26[C] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | ZA | 26[D] | GLN |
| 15 | ZA | 26[E] | GLN |
| 15 | ZA | 26[F] | GLN |
| 15 | ZA | 46[A] | HIS |
| 15 | ZA | 46[B] | HIS |
| 15 | ZA | 46[C] | HIS |
| 15 | ZA | 46[D] | HIS |
| 15 | ZA | 46[E] | HIS |
| 15 | ZA | 46[F] | HIS |
| 15 | ZA | 50[A] | LYS |
| 15 | ZA | 50[B] | LYS |
| 15 | ZA | 50[C] | LYS |
| 15 | ZA | 50[D] | LYS |
| 15 | ZA | 50[E] | LYS |
| 15 | ZA | 50[F] | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (602) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 63 | ASN |
| 1 | A | 159 | ASN |
| 1 | A | 246 | ASN |
| 1 | A | 255 | ASN |
| 1 | A | 303 | ASN |
| 1 | A | 434 | GLN |
| 1 | A | 490 | ASN |
| 1 | A | 644 | ASN |
| 1 | B | 69 | GLN |
| 1 | B | 84 | ASN |
| 1 | B | 196 | GLN |
| 1 | B | 336 | GLN |
| 1 | B | 388 | GLN |
| 1 | B | 568 | ASN |
| 1 | B | 570 | GLN |
| 1 | B | 582 | ASN |
| 2 | C | 87 | GLN |
| 2 | C | 91 | GLN |
| 2 | C | 139 | ASN |
| 2 | C | 528 | ASN |
| 2 | C | 601 | ASN |
| 2 | C | 663 | ASN |
| 2 | C | 673 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 682 | GLN |
| 2 | C | 684 | ASN |
| 2 | C | 688 | ASN |
| 2 | C | 908 | HIS |
| 2 | C | 914 | ASN |
| 3 | E | 23 | ASN |
| 3 | E | 201 | ASN |
| 3 | E | 271 | GLN |
| 3 | E | 314 | ASN |
| 4 | F | 29 | ASN |
| 4 | F | 70 | HIS |
| 4 | F | 111 | ASN |
| 4 | F | 120 | ASN |
| 4 | G | 29 | ASN |
| 4 | G | 70 | HIS |
| 4 | G | 111 | ASN |
| 4 | G | 120 | ASN |
| 4 | H | 29 | ASN |
| 4 | H | 70 | HIS |
| 4 | H | 111 | ASN |
| 4 | H | 120 | ASN |
| 5 | I | 209 | ASN |
| 5 | I | 307 | ASN |
| 5 | I | 382 | ASN |
| 5 | I | 388 | ASN |
| 5 | I | 483 | GLN |
| 5 | J | 161 | ASN |
| 5 | J | 198 | ASN |
| 5 | J | 305 | ASN |
| 5 | J | 382 | ASN |
| 5 | J | 440 | GLN |
| 5 | J | 504 | ASN |
| 5 | J | 514 | HIS |
| 5 | K | 127 | ASN |
| 5 | K | 150 | GLN |
| 5 | K | 198 | ASN |
| 5 | K | 305 | ASN |
| 5 | K | 318 | GLN |
| 5 | K | 377 | HIS |
| 5 | K | 410 | GLN |
| 5 | K | 421 | ASN |
| 5 | K | 440 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | K | 444 | ASN |
| 5 | K | 483 | GLN |
| 5 | K | 498 | ASN |
| 5 | K | 504 | ASN |
| 6 | L | 31 | ASN |
| 6 | L | 164 | GLN |
| 6 | M | 31 | ASN |
| 6 | M | 164 | GLN |
| 6 | M | 205 | ASN |
| 6 | N | 31 | ASN |
| 6 | N | 164 | GLN |
| 7 | O | 24 | ASN |
| 7 | O | 233 | GLN |
| 7 | O | 389 | ASN |
| 7 | O | 441 | GLN |
| 7 | O | 520 | ASN |
| 7 | P | 111 | ASN |
| 7 | P | 166 | GLN |
| 7 | P | 167 | GLN |
| 7 | P | 233 | GLN |
| 7 | P | 327 | GLN |
| 7 | P | 329 | ASN |
| 7 | P | 389 | ASN |
| 7 | Q | 3 | ASN |
| 7 | Q | 139 | ASN |
| 7 | Q | 217 | ASN |
| 7 | Q | 233 | GLN |
| 8 | R | 83 | GLN |
| 8 | R | 151 | GLN |
| 8 | S | 83 | GLN |
| 8 | S | 151 | GLN |
| 10 | U | 337 | ASN |
| 11 | V | 182 | ASN |
| 12 | W | 175 | GLN |
| 12 | W | 211 | HIS |
| 1 | X | 63 | ASN |
| 1 | X | 69 | GLN |
| 1 | X | 159 | ASN |
| 1 | X | 246 | ASN |
| 1 | X | 255 | ASN |
| 1 | X | 303 | ASN |
| 1 | X | 434 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | X | 490 | ASN |
| 1 | X | 644 | ASN |
| 1 | Y | 69 | GLN |
| 1 | Y | 84 | ASN |
| 1 | Y | 196 | GLN |
| 1 | Y | 336 | GLN |
| 1 | Y | 388 | GLN |
| 1 | Y | 568 | ASN |
| 1 | Y | 570 | GLN |
| 1 | Y | 582 | ASN |
| 2 | Z | 87 | GLN |
| 2 | Z | 91 | GLN |
| 2 | Z | 139 | ASN |
| 2 | Z | 528 | ASN |
| 2 | Z | 601 | ASN |
| 2 | Z | 663 | ASN |
| 2 | Z | 673 | GLN |
| 2 | Z | 682 | GLN |
| 2 | Z | 684 | ASN |
| 2 | Z | 688 | ASN |
| 2 | Z | 908 | HIS |
| 2 | Z | 914 | ASN |
| 3 | b | 23 | ASN |
| 3 | b | 201 | ASN |
| 3 | b | 271 | GLN |
| 3 | b | 314 | ASN |
| 4 | c | 29 | ASN |
| 4 | c | 70 | HIS |
| 4 | c | 111 | ASN |
| 4 | c | 120 | ASN |
| 4 | d | 29 | ASN |
| 4 | d | 70 | HIS |
| 4 | d | 111 | ASN |
| 4 | d | 120 | ASN |
| 4 | d | 155 | ASN |
| 4 | e | 29 | ASN |
| 4 | e | 70 | HIS |
| 4 | e | 111 | ASN |
| 4 | e | 120 | ASN |
| 5 | f | 209 | ASN |
| 5 | f | 307 | ASN |
| 5 | f | 382 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | f | 388 | ASN |
| 5 | f | 483 | GLN |
| 5 | g | 161 | ASN |
| 5 | g | 198 | ASN |
| 5 | g | 305 | ASN |
| 5 | g | 382 | ASN |
| 5 | g | 440 | GLN |
| 5 | g | 504 | ASN |
| 5 | g | 514 | HIS |
| 5 | g | 588 | ASN |
| 5 | h | 127 | ASN |
| 5 | h | 150 | GLN |
| 5 | h | 198 | ASN |
| 5 | h | 305 | ASN |
| 5 | h | 318 | GLN |
| 5 | h | 377 | HIS |
| 5 | h | 410 | GLN |
| 5 | h | 421 | ASN |
| 5 | h | 440 | GLN |
| 5 | h | 444 | ASN |
| 5 | h | 483 | GLN |
| 5 | h | 498 | ASN |
| 5 | h | 504 | ASN |
| 6 | i | 31 | ASN |
| 6 | i | 164 | GLN |
| 6 | j | 31 | ASN |
| 6 | j | 205 | ASN |
| 6 | k | 31 | ASN |
| 6 | k | 164 | GLN |
| 7 | l | 24 | ASN |
| 7 | l | 233 | GLN |
| 7 | l | 389 | ASN |
| 7 | l | 441 | GLN |
| 7 | l | 520 | ASN |
| 7 | m | 111 | ASN |
| 7 | m | 166 | GLN |
| 7 | m | 167 | GLN |
| 7 | m | 233 | GLN |
| 7 | m | 327 | GLN |
| 7 | m | 329 | ASN |
| 7 | m | 389 | ASN |
| 7 | n | 3 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | n | 139 | ASN |
| 7 | n | 217 | ASN |
| 7 | n | 233 | GLN |
| 8 | o | 83 | GLN |
| 8 | o | 151 | GLN |
| 8 | p | 83 | GLN |
| 8 | p | 151 | GLN |
| 11 | s | 182 | ASN |
| 12 | t | 175 | GLN |
| 12 | t | 211 | HIS |
| 1 | u | 63 | ASN |
| 1 | u | 69 | GLN |
| 1 | u | 159 | ASN |
| 1 | u | 246 | ASN |
| 1 | u | 255 | ASN |
| 1 | u | 303 | ASN |
| 1 | u | 434 | GLN |
| 1 | u | 490 | ASN |
| 1 | u | 644 | ASN |
| 1 | v | 69 | GLN |
| 1 | v | 84 | ASN |
| 1 | v | 196 | GLN |
| 1 | v | 336 | GLN |
| 1 | v | 388 | GLN |
| 1 | v | 568 | ASN |
| 1 | v | 570 | GLN |
| 1 | v | 582 | ASN |
| 2 | w | 87 | GLN |
| 2 | w | 91 | GLN |
| 2 | w | 139 | ASN |
| 2 | w | 528 | ASN |
| 2 | w | 601 | ASN |
| 2 | w | 663 | ASN |
| 2 | w | 673 | GLN |
| 2 | w | 682 | GLN |
| 2 | w | 684 | ASN |
| 2 | w | 688 | ASN |
| 2 | w | 908 | HIS |
| 2 | w | 914 | ASN |
| 3 | y | 23 | ASN |
| 3 | y | 201 | ASN |
| 3 | y | 271 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | y | 314 | ASN |
| 4 | z | 29 | ASN |
| 4 | z | 70 | HIS |
| 4 | z | 111 | ASN |
| 4 | z | 120 | ASN |
| 4 | AA | 29 | ASN |
| 4 | AA | 70 | HIS |
| 4 | AA | 111 | ASN |
| 4 | AA | 120 | ASN |
| 4 | AB | 29 | ASN |
| 4 | AB | 70 | HIS |
| 4 | AB | 111 | ASN |
| 4 | AB | 120 | ASN |
| 5 | AC | 209 | ASN |
| 5 | AC | 307 | ASN |
| 5 | AC | 382 | ASN |
| 5 | AC | 388 | ASN |
| 5 | AC | 483 | GLN |
| 5 | AD | 161 | ASN |
| 5 | AD | 198 | ASN |
| 5 | AD | 305 | ASN |
| 5 | AD | 382 | ASN |
| 5 | AD | 440 | GLN |
| 5 | AD | 504 | ASN |
| 5 | AD | 514 | HIS |
| 5 | AD | 588 | ASN |
| 5 | AE | 127 | ASN |
| 5 | AE | 150 | GLN |
| 5 | AE | 198 | ASN |
| 5 | AE | 305 | ASN |
| 5 | AE | 318 | GLN |
| 5 | AE | 377 | HIS |
| 5 | AE | 410 | GLN |
| 5 | AE | 421 | ASN |
| 5 | AE | 440 | GLN |
| 5 | AE | 444 | ASN |
| 5 | AE | 483 | GLN |
| 5 | AE | 498 | ASN |
| 5 | AE | 504 | ASN |
| 6 | AF | 31 | ASN |
| 6 | AF | 164 | GLN |
| 6 | AG | 31 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | AG | 205 | ASN |
| 6 | AH | 31 | ASN |
| 6 | AH | 164 | GLN |
| 7 | AI | 24 | ASN |
| 7 | AI | 233 | GLN |
| 7 | AI | 389 | ASN |
| 7 | AI | 441 | GLN |
| 7 | AI | 520 | ASN |
| 7 | AJ | 111 | ASN |
| 7 | AJ | 166 | GLN |
| 7 | AJ | 167 | GLN |
| 7 | AJ | 233 | GLN |
| 7 | AJ | 327 | GLN |
| 7 | AJ | 329 | ASN |
| 7 | AJ | 389 | ASN |
| 7 | BA | 3 | ASN |
| 7 | BA | 139 | ASN |
| 7 | BA | 217 | ASN |
| 7 | BA | 233 | GLN |
| 8 | BB | 83 | GLN |
| 8 | BB | 151 | GLN |
| 8 | BC | 83 | GLN |
| 8 | BC | 151 | GLN |
| 10 | BE | 337 | ASN |
| 11 | BF | 182 | ASN |
| 12 | BG | 175 | GLN |
| 12 | BG | 211 | HIS |
| 1 | BH | 63 | ASN |
| 1 | BH | 69 | GLN |
| 1 | BH | 159 | ASN |
| 1 | BH | 246 | ASN |
| 1 | BH | 255 | ASN |
| 1 | BH | 303 | ASN |
| 1 | BH | 434 | GLN |
| 1 | BH | 490 | ASN |
| 1 | BH | 644 | ASN |
| 1 | BI | 69 | GLN |
| 1 | BI | 84 | ASN |
| 1 | BI | 196 | GLN |
| 1 | BI | 336 | GLN |
| 1 | BI | 388 | GLN |
| 1 | BI | 568 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BI | 570 | GLN |
| 1 | BI | 582 | ASN |
| 2 | BJ | 87 | GLN |
| 2 | BJ | 91 | GLN |
| 2 | BJ | 139 | ASN |
| 2 | BJ | 528 | ASN |
| 2 | BJ | 663 | ASN |
| 2 | BJ | 673 | GLN |
| 2 | BJ | 682 | GLN |
| 2 | BJ | 684 | ASN |
| 2 | BJ | 688 | ASN |
| 2 | BJ | 908 | HIS |
| 2 | BJ | 914 | ASN |
| 3 | CB | 23 | ASN |
| 3 | CB | 201 | ASN |
| 3 | CB | 271 | GLN |
| 3 | CB | 314 | ASN |
| 4 | CC | 29 | ASN |
| 4 | CC | 70 | HIS |
| 4 | CC | 111 | ASN |
| 4 | CC | 120 | ASN |
| 4 | CD | 29 | ASN |
| 4 | CD | 70 | HIS |
| 4 | CD | 111 | ASN |
| 4 | CD | 120 | ASN |
| 4 | CE | 29 | ASN |
| 4 | CE | 70 | HIS |
| 4 | CE | 120 | ASN |
| 5 | CF | 209 | ASN |
| 5 | CF | 307 | ASN |
| 5 | CF | 382 | ASN |
| 5 | CF | 388 | ASN |
| 5 | CF | 483 | GLN |
| 5 | CG | 161 | ASN |
| 5 | CG | 198 | ASN |
| 5 | CG | 305 | ASN |
| 5 | CG | 382 | ASN |
| 5 | CG | 440 | GLN |
| 5 | CG | 504 | ASN |
| 5 | CG | 514 | HIS |
| 5 | CG | 588 | ASN |
| 5 | CH | 127 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | CH | 150 | GLN |
| 5 | CH | 198 | ASN |
| 5 | CH | 305 | ASN |
| 5 | CH | 318 | GLN |
| 5 | CH | 377 | HIS |
| 5 | CH | 410 | GLN |
| 5 | CH | 421 | ASN |
| 5 | CH | 440 | GLN |
| 5 | CH | 444 | ASN |
| 5 | CH | 483 | GLN |
| 5 | CH | 498 | ASN |
| 5 | CH | 504 | ASN |
| 6 | CI | 31 | ASN |
| 6 | CI | 164 | GLN |
| 6 | CJ | 31 | ASN |
| 6 | CJ | 164 | GLN |
| 6 | CJ | 205 | ASN |
| 6 | DA | 31 | ASN |
| 6 | DA | 164 | GLN |
| 7 | DB | 24 | ASN |
| 7 | DB | 233 | GLN |
| 7 | DB | 389 | ASN |
| 7 | DB | 441 | GLN |
| 7 | DB | 520 | ASN |
| 7 | DC | 111 | ASN |
| 7 | DC | 166 | GLN |
| 7 | DC | 167 | GLN |
| 7 | DC | 233 | GLN |
| 7 | DC | 327 | GLN |
| 7 | DC | 329 | ASN |
| 7 | DC | 389 | ASN |
| 7 | DD | 3 | ASN |
| 7 | DD | 139 | ASN |
| 7 | DD | 217 | ASN |
| 7 | DD | 233 | GLN |
| 8 | DE | 83 | GLN |
| 8 | DE | 151 | GLN |
| 8 | DF | 83 | GLN |
| 8 | DF | 151 | GLN |
| 11 | DI | 182 | ASN |
| 12 | DJ | 175 | GLN |
| 12 | DJ | 211 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | EA | 63 | ASN |
| 1 | EA | 69 | GLN |
| 1 | EA | 159 | ASN |
| 1 | EA | 246 | ASN |
| 1 | EA | 255 | ASN |
| 1 | EA | 303 | ASN |
| 1 | EA | 434 | GLN |
| 1 | EA | 490 | ASN |
| 1 | EA | 644 | ASN |
| 1 | EB | 69 | GLN |
| 1 | EB | 84 | ASN |
| 1 | EB | 196 | GLN |
| 1 | EB | 336 | GLN |
| 1 | EB | 388 | GLN |
| 1 | EB | 568 | ASN |
| 1 | EB | 570 | GLN |
| 1 | EB | 582 | ASN |
| 2 | EC | 87 | GLN |
| 2 | EC | 91 | GLN |
| 2 | EC | 139 | ASN |
| 2 | EC | 528 | ASN |
| 2 | EC | 663 | ASN |
| 2 | EC | 673 | GLN |
| 2 | EC | 682 | GLN |
| 2 | EC | 908 | HIS |
| 2 | EC | 914 | ASN |
| 3 | EE | 23 | ASN |
| 3 | EE | 201 | ASN |
| 3 | EE | 271 | GLN |
| 3 | EE | 314 | ASN |
| 4 | EF | 29 | ASN |
| 4 | EF | 70 | HIS |
| 4 | EF | 111 | ASN |
| 4 | EF | 120 | ASN |
| 4 | EG | 29 | ASN |
| 4 | EG | 70 | HIS |
| 4 | EG | 111 | ASN |
| 4 | EG | 120 | ASN |
| 4 | EG | 155 | ASN |
| 4 | EH | 29 | ASN |
| 4 | EH | 70 | HIS |
| 4 | EH | 120 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | EI | 209 | ASN |
| 5 | EI | 307 | ASN |
| 5 | EI | 382 | ASN |
| 5 | EI | 388 | ASN |
| 5 | EI | 483 | GLN |
| 5 | EI | 588 | ASN |
| 5 | EJ | 161 | ASN |
| 5 | EJ | 198 | ASN |
| 5 | EJ | 305 | ASN |
| 5 | EJ | 382 | ASN |
| 5 | EJ | 440 | GLN |
| 5 | EJ | 504 | ASN |
| 5 | EJ | 514 | HIS |
| 5 | FA | 127 | ASN |
| 5 | FA | 150 | GLN |
| 5 | FA | 198 | ASN |
| 5 | FA | 305 | ASN |
| 5 | FA | 318 | GLN |
| 5 | FA | 377 | HIS |
| 5 | FA | 410 | GLN |
| 5 | FA | 421 | ASN |
| 5 | FA | 440 | GLN |
| 5 | FA | 444 | ASN |
| 5 | FA | 483 | GLN |
| 5 | FA | 498 | ASN |
| 5 | FA | 504 | ASN |
| 6 | FB | 164 | GLN |
| 6 | FC | 31 | ASN |
| 6 | FC | 164 | GLN |
| 6 | FC | 205 | ASN |
| 6 | FD | 31 | ASN |
| 6 | FD | 164 | GLN |
| 7 | FE | 24 | ASN |
| 7 | FE | 233 | GLN |
| 7 | FE | 389 | ASN |
| 7 | FE | 441 | GLN |
| 7 | FE | 520 | ASN |
| 7 | FF | 111 | ASN |
| 7 | FF | 167 | GLN |
| 7 | FF | 233 | GLN |
| 7 | FF | 327 | GLN |
| 7 | FF | 329 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | FF | 389 | ASN |
| 7 | FG | 3 | ASN |
| 7 | FG | 139 | ASN |
| 7 | FG | 217 | ASN |
| 7 | FG | 233 | GLN |
| 8 | FH | 83 | GLN |
| 8 | FH | 151 | GLN |
| 8 | FI | 83 | GLN |
| 8 | FI | 115 | GLN |
| 8 | FI | 151 | GLN |
| 10 | GA | 337 | ASN |
| 11 | GB | 182 | ASN |
| 12 | GC | 175 | GLN |
| 12 | GC | 211 | HIS |
| 1 | GD | 63 | ASN |
| 1 | GD | 69 | GLN |
| 1 | GD | 159 | ASN |
| 1 | GD | 246 | ASN |
| 1 | GD | 255 | ASN |
| 1 | GD | 303 | ASN |
| 1 | GD | 434 | GLN |
| 1 | GD | 490 | ASN |
| 1 | GD | 644 | ASN |
| 1 | GE | 69 | GLN |
| 1 | GE | 84 | ASN |
| 1 | GE | 196 | GLN |
| 1 | GE | 336 | GLN |
| 1 | GE | 388 | GLN |
| 1 | GE | 568 | ASN |
| 1 | GE | 570 | GLN |
| 1 | GE | 582 | ASN |
| 2 | GF | 87 | GLN |
| 2 | GF | 91 | GLN |
| 2 | GF | 139 | ASN |
| 2 | GF | 333 | ASN |
| 2 | GF | 528 | ASN |
| 2 | GF | 663 | ASN |
| 2 | GF | 673 | GLN |
| 2 | GF | 682 | GLN |
| 2 | GF | 684 | ASN |
| 2 | GF | 688 | ASN |
| 2 | GF | 908 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | GF | 914 | ASN |
| 3 | GH | 23 | ASN |
| 3 | GH | 201 | ASN |
| 3 | GH | 271 | GLN |
| 3 | GH | 314 | ASN |
| 4 | GI | 29 | ASN |
| 4 | GI | 70 | HIS |
| 4 | GI | 111 | ASN |
| 4 | GI | 120 | ASN |
| 4 | GJ | 29 | ASN |
| 4 | GJ | 70 | HIS |
| 4 | GJ | 111 | ASN |
| 4 | GJ | 120 | ASN |
| 4 | GJ | 155 | ASN |
| 4 | HA | 29 | ASN |
| 4 | HA | 70 | HIS |
| 4 | HA | 111 | ASN |
| 4 | HA | 120 | ASN |
| 5 | HB | 209 | ASN |
| 5 | HB | 307 | ASN |
| 5 | HB | 388 | ASN |
| 5 | HB | 483 | GLN |
| 5 | HB | 588 | ASN |
| 5 | HC | 161 | ASN |
| 5 | HC | 198 | ASN |
| 5 | HC | 305 | ASN |
| 5 | HC | 382 | ASN |
| 5 | HC | 440 | GLN |
| 5 | HC | 504 | ASN |
| 5 | HC | 514 | HIS |
| 5 | HD | 127 | ASN |
| 5 | HD | 150 | GLN |
| 5 | HD | 198 | ASN |
| 5 | HD | 305 | ASN |
| 5 | HD | 318 | GLN |
| 5 | HD | 377 | HIS |
| 5 | HD | 410 | GLN |
| 5 | HD | 421 | ASN |
| 5 | HD | 440 | GLN |
| 5 | HD | 444 | ASN |
| 5 | HD | 483 | GLN |
| 5 | HD | 498 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | HD | 504 | ASN |
| 6 | HE | 31 | ASN |
| 6 | HE | 164 | GLN |
| 6 | HF | 31 | ASN |
| 6 | HF | 164 | GLN |
| 6 | HF | 205 | ASN |
| 6 | HG | 31 | ASN |
| 6 | HG | 164 | GLN |
| 7 | HH | 24 | ASN |
| 7 | HH | 233 | GLN |
| 7 | HH | 389 | ASN |
| 7 | HH | 441 | GLN |
| 7 | HH | 520 | ASN |
| 7 | HI | 111 | ASN |
| 7 | HI | 166 | GLN |
| 7 | HI | 167 | GLN |
| 7 | HI | 233 | GLN |
| 7 | HI | 327 | GLN |
| 7 | HI | 329 | ASN |
| 7 | HI | 389 | ASN |
| 7 | HJ | 3 | ASN |
| 7 | HJ | 139 | ASN |
| 7 | HJ | 217 | ASN |
| 7 | HJ | 233 | GLN |
| 8 | IA | 83 | GLN |
| 8 | IA | 151 | GLN |
| 8 | IB | 83 | GLN |
| 8 | IB | 115 | GLN |
| 8 | IB | 151 | GLN |
| 9 | IC | 83 | ASN |
| 11 | IE | 182 | ASN |
| 12 | IF | 175 | GLN |
| 12 | IF | 211 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 13 | YA | 17 |
| 13 | YC | 17 |
| 13 | YB | 17 |
| 14 | YD | 5 |
| 14 | YF | 5 |
| 15 | ZA | 5 |
| 14 | YE | 5 |
| 2 | GF | 1 |
| 5 | g | 1 |
| 7 | BA | 1 |
| 3 | CA | 1 |
| 1 | B | 1 |
| 1 | EB | 1 |
| 3 | GG | 1 |
| 3 | D | 1 |
| 1 | GE | 1 |

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| Mol | Chain | Number of breaks |
|---|---|---|
| 7 | DD | 1 |
| 5 | J | 1 |
| 7 | HJ | 1 |
| 1 | BI | 1 |
| 2 | w | 1 |
| 7 | n | 1 |
| 3 | x | 1 |
| 2 | BJ | 1 |
| 5 | CG | 1 |
| 5 | AD | 1 |
| 1 | v | 1 |
| 2 | Z | 1 |
| 3 | a | 1 |
| 5 | HC | 1 |
| 7 | Q | 1 |
| 3 | ED | 1 |
| 2 | C | 1 |
| 7 | FG | 1 |
| 2 | EC | 1 |
| 1 | Y | 1 |
| 5 | EJ | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | YA | 76[E]:PRO | C | 77[E]:VAL | N | 10.44 |
| 1 | YB | 76[E]:PRO | C | 77[E]:VAL | N | 10.44 |
| 1 | YC | 76[E]:PRO | C | 77[E]:VAL | N | 10.44 |
| 1 | YC | 76[B]:PRO | C | 77[B]:VAL | N | 9.41 |
| 1 | YA | 76[B]:PRO | C | 77[B]:VAL | N | 9.40 |
| 1 | YB | 76[B]:PRO | C | 77[B]:VAL | N | 9.40 |
| 1 | YA | 76[C]:PRO | C | 77[C]:VAL | N | 9.29 |
| 1 | YB | 76[C]:PRO | C | 77[C]:VAL | N | 9.29 |
| 1 | YC | 76[C]:PRO | C | 77[C]:VAL | N | 9.29 |
| 1 | YA | 76[F]:PRO | C | 77[F]:VAL | N | 9.21 |
| 1 | YB | 76[F]:PRO | C | 77[F]:VAL | N | 9.21 |
| 1 | YC | 76[F]:PRO | C | 77[F]:VAL | N | 9.21 |
| 1 | YA | 76[A]:PRO | C | 77[A]:VAL | N | 9.00 |
| 1 | YA | 76[D]:PRO | C | 77[D]:VAL | N | 9.00 |
| 1 | YB | 76[A]:PRO | C | 77[A]:VAL | N | 9.00 |
| 1 | YB | 76[D]:PRO | C | 77[D]:VAL | N | 9.00 |
| 1 | YC | 76[A]:PRO | C | 77[A]:VAL | N | 9.00 |
| 1 | YC | 76[D]:PRO | C | 77[D]:VAL | N | 9.00 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | YA | 112[A]:GLU | C | 113[A]:GLY | N | 3.79 |
| 1 | YA | 112[B]:GLU | C | 113[B]:GLY | N | 3.79 |
| 1 | YA | 112[D]:GLU | C | 113[D]:GLY | N | 3.79 |
| 1 | YA | 112[E]:GLU | C | 113[E]:GLY | N | 3.79 |
| 1 | YB | 112[A]:GLU | C | 113[A]:GLY | N | 3.79 |
| 1 | YB | 112[B]:GLU | C | 113[B]:GLY | N | 3.79 |
| 1 | YB | 112[D]:GLU | C | 113[D]:GLY | N | 3.79 |
| 1 | YB | 112[E]:GLU | C | 113[E]:GLY | N | 3.79 |
| 1 | YC | 112[A]:GLU | C | 113[A]:GLY | N | 3.79 |
| 1 | YC | 112[B]:GLU | C | 113[B]:GLY | N | 3.79 |
| 1 | YC | 112[D]:GLU | C | 113[D]:GLY | N | 3.79 |
| 1 | YC | 112[E]:GLU | C | 113[E]:GLY | N | 3.79 |
| 1 | YA | 112[C]:GLU | C | 113[C]:GLY | N | 3.78 |
| 1 | YA | 112[F]:GLU | C | 113[F]:GLY | N | 3.78 |
| 1 | YB | 112[C]:GLU | C | 113[C]:GLY | N | 3.78 |
| 1 | YB | 112[F]:GLU | C | 113[F]:GLY | N | 3.78 |
| 1 | YC | 112[C]:GLU | C | 113[C]:GLY | N | 3.78 |
| 1 | YC | 112[F]:GLU | C | 113[F]:GLY | N | 3.78 |
| 1 | YA | 574[B]:ILE | C | 575[B]:GLY | N | 3.02 |
| 1 | YA | 574[C]:ILE | C | 575[C]:GLY | N | 3.02 |
| 1 | YA | 574[D]:ILE | C | 575[D]:GLY | N | 3.02 |
| 1 | YA | 574[E]:ILE | C | 575[E]:GLY | N | 3.02 |
| 1 | YA | 574[F]:ILE | C | 575[F]:GLY | N | 3.02 |
| 1 | YB | 574[B]:ILE | C | 575[B]:GLY | N | 3.02 |
| 1 | YB | 574[C]:ILE | C | 575[C]:GLY | N | 3.02 |
| 1 | YB | 574[D]:ILE | C | 575[D]:GLY | N | 3.02 |
| 1 | YB | 574[E]:ILE | C | 575[E]:GLY | N | 3.02 |
| 1 | YB | 574[F]:ILE | C | 575[F]:GLY | N | 3.02 |
| 1 | YC | 574[B]:ILE | C | 575[B]:GLY | N | 3.02 |
| 1 | YC | 574[C]:ILE | C | 575[C]:GLY | N | 3.02 |
| 1 | YC | 574[D]:ILE | C | 575[D]:GLY | N | 3.02 |
| 1 | YC | 574[E]:ILE | C | 575[E]:GLY | N | 3.02 |
| 1 | YC | 574[F]:ILE | C | 575[F]:GLY | N | 3.02 |
| 1 | ZA | 96[B]:ILE | C | 97[B]:LYS | N | 2.95 |
| 1 | ZA | 96[E]:ILE | C | 97[E]:LYS | N | 2.95 |
| 1 | ZA | 96[C]:ILE | C | 97[C]:LYS | N | 2.94 |
| 1 | ZA | 96[D]:ILE | C | 97[D]:LYS | N | 2.94 |
| 1 | ZA | 96[F]:ILE | C | 97[F]:LYS | N | 2.94 |
| 1 | YD | 375[B]:GLU | C | 376[B]:PHE | N | 2.90 |
| 1 | YD | 375[C]:GLU | C | 376[C]:PHE | N | 2.90 |
| 1 | YD | 375[D]:GLU | C | 376[D]:PHE | N | 2.90 |
| 1 | YD | 375[E]:GLU | C | 376[E]:PHE | N | 2.90 |

*Continued on next page...*

*Continued from previous page...*

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | YD | 375[F]:GLU | C | 376[F]:PHE | N | 2.90 |
| 1 | YE | 375[B]:GLU | C | 376[B]:PHE | N | 2.90 |
| 1 | YE | 375[C]:GLU | C | 376[C]:PHE | N | 2.90 |
| 1 | YE | 375[D]:GLU | C | 376[D]:PHE | N | 2.90 |
| 1 | YE | 375[E]:GLU | C | 376[E]:PHE | N | 2.90 |
| 1 | YE | 375[F]:GLU | C | 376[F]:PHE | N | 2.90 |
| 1 | YF | 375[B]:GLU | C | 376[B]:PHE | N | 2.90 |
| 1 | YF | 375[C]:GLU | C | 376[C]:PHE | N | 2.90 |
| 1 | YF | 375[D]:GLU | C | 376[D]:PHE | N | 2.90 |
| 1 | YF | 375[E]:GLU | C | 376[E]:PHE | N | 2.90 |
| 1 | YF | 375[F]:GLU | C | 376[F]:PHE | N | 2.90 |
| 1 | CG | 531:ASN | C | 532:LEU | N | 1.19 |
| 1 | EJ | 531:ASN | C | 532:LEU | N | 1.19 |
| 1 | J | 531:ASN | C | 532:LEU | N | 1.18 |
| 1 | Q | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | g | 531:ASN | C | 532:LEU | N | 1.18 |
| 1 | n | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | AD | 531:ASN | C | 532:LEU | N | 1.18 |
| 1 | BA | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | DD | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | FG | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | HC | 531:ASN | C | 532:LEU | N | 1.18 |
| 1 | HJ | 26:PRO | C | 27:PRO | N | 1.18 |
| 1 | B | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | C | 652:MET | C | 653:MET | N | 1.10 |
| 1 | Y | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | Z | 652:MET | C | 653:MET | N | 1.10 |
| 1 | v | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | w | 652:MET | C | 653:MET | N | 1.10 |
| 1 | BI | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | BJ | 652:MET | C | 653:MET | N | 1.10 |
| 1 | EB | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | EC | 652:MET | C | 653:MET | N | 1.10 |
| 1 | GE | 307:ASP | C | 308:PRO | N | 1.10 |
| 1 | GF | 652:MET | C | 653:MET | N | 1.10 |
| 1 | D | 258:PHE | C | 259:PRO | N | 0.94 |
| 1 | a | 258:PHE | C | 259:PRO | N | 0.94 |
| 1 | x | 258:PHE | C | 259:PRO | N | 0.94 |
| 1 | CA | 258:PHE | C | 259:PRO | N | 0.94 |
| 1 | ED | 258:PHE | C | 259:PRO | N | 0.94 |
| 1 | GG | 258:PHE | C | 259:PRO | N | 0.94 |